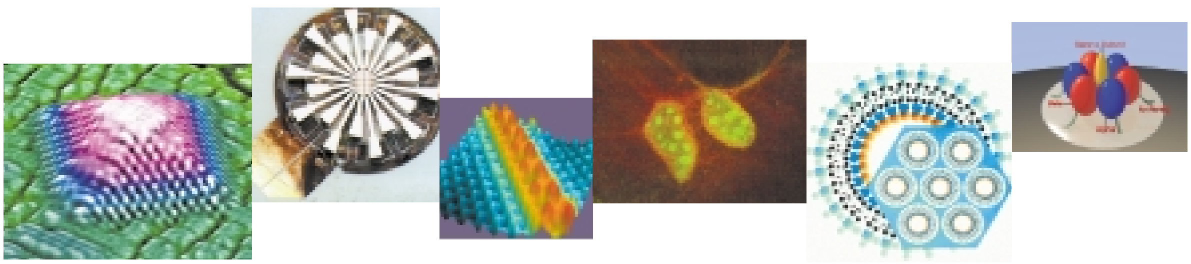
National Nanotechnology Initiative

The Initiative and its Implementation Plan



National Science and Technology Council
Committee on Technology
Subcommittee on Nanoscale Science, Engineering and Technology

July 2000

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About the National Science and Technology Council

President Clinton established the National Science and Technology Council (NSTC) by Executive Order on November 23, 1993. This cabinet-level council is the principal means for the President to coordinate science, space and technology policies across the Federal Government. NSTC acts as a "virtual" agency for science and technology (S&T). The President chairs the NSTC. Membership consists of the Vice President, Assistant to the President for Science and Technology, Cabinet Secretaries and Agency Heads with significant S&T responsibilities, and other White House officials.

Through the NSTC, Federal departments and agencies work cooperatively to ensure that Federal science and technology investments support national goals. NSTC Committees prepare R&D strategies that are coordinated across the Federal government to form a comprehensive investment package.

Call (202)456-6100 to obtain additional information regarding the NSTC.

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Call (202)456-7116 to obtain additional information regarding the OSTP, or visit the OSTP web site at: http://www.whitehouse.gov/WH/EOP/OSTP/html/OSTP_Home.html

About the cover: The cover contains a collection of images that represent the nanotechnology research and development activities currently underway among the Federal Agencies participating in the NNI. From left to right: a self-assembled germanium pyramid that is 10 nm in size (NSF); nanoscale devices and sensors to help characterize space exploration (NASA); field-assisted assembly of cesium atoms on a GaAs substrate (NIST); visualization of human tissues using semiconductor nanocrystals (DOE); chemically selective surfactant molecules showing numerous environmental and commercial (DOE); and naturally-occurring molecular biomotors powered by biochemical processes (NSF).

NATIONAL NANOTECHNOLOGY INITIATIVE:

The Initiative and Its Implementation Plan

National Science and Technology Council
Committee on Technology
Subcommittee on Nanoscale Science, Engineering and Technology

July 2000
Washington, D.C.

THE WHITE HOUSE

July 11, 2000

MEMBERS OF CONGRESS:

I am pleased to forward with this letter the *National Nanotechnology Initiative: The Initiative and Its Implementation Plan*. The report was prepared by the National Science and Technology Council's Committee on Technology, Subcommittee on Nanoscale Science Engineering and Technology (NSET). This new NSET Subcommittee succeeds the Interagency Working Group on Nanoscience, Engineering, and Technology (IWGN) as the primary interagency coordination mechanism. This report builds upon the *National Nanotechnology Initiative: Leading to the Next Industrial Revolution* included as a Supplement to the President's FY 2001 Budget.

The President has made the National Nanotechnology Initiative (NNI) a top priority. Nanotechnology thrives from modern advances in chemistry, physics, biology, engineering, medical, and materials research and will contribute to cross-disciplinary training of the 21st century science and technology workforce. The Administration believes that nanotechnology will have a profound impact on our economy and society in the early 21st century, perhaps comparable to that of information technology or of cellular, genetic, and molecular biology.

In the FY 2001 budget, the President proposes to expand the Federal nanotechnology investment portfolio with this initiative, nearly doubling the current Federal research in nanotechnology to $495 million. The NNI incorporates fundamental research, Grand Challenges, centers and networks of excellence and research infrastructure, as well as ethical, legal and social implications and workforce.

The President's Committee of Advisers on Science and Technology (PCAST) strongly endorsed the establishment of the NNI. With PCAST's recommendation, the President is taking the vital first step to increase funding for long-term, high-risk R&D that will allow our nation to move to the forefront of the nanotechnology frontier.

The Administration looks forward to working with Congress to strengthen investments in nanotechnology research. Only by working in a bipartisan manner can we further solidify the technological base that lies at the heart of America's scientific and economic leadership.

Sincerely,

Neal Lane

Neal Lane
Assistant to the President
for Science and Technology

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EXECUTIVE SUMMARY

> "My budget supports a major new National Nanotechnology Initiative, worth $500 million. … the ability to manipulate matter at the atomic and molecular level. Imagine the possibilities: materials with ten times the strength of steel and only a small fraction of the weight -- shrinking all the information housed at the Library of Congress into a device the size of a sugar cube -- detecting cancerous tumors when they are only a few cells in size. Some of our research goals may take 20 or more years to achieve, but that is precisely why there is an important role for the federal government."

--President William J. Clinton
January 21, 2000
California Institute of Technology

President Clinton's (fiscal year) FY 2001 budget request includes a $225 million (83%) increase in the federal government's investment in nanotechnology research and development. The Administration has made the National Nanotechnology Initiative (NNI) a top science and technology priority. The emerging fields of nanoscience and nanoengineering – the ability to work at the molecular level, atom by atom, to create large structures with fundamentally new molecular organization - are leading to unprecedented understanding and control over the fundamental building blocks of all physical things. The nanoscale is not just another step towards miniaturization. Compared to the physical properties and behavior of isolated molecules or bulk materials, materials with structural features in the ranges of 1 to 100 nanometers – 100 to 10,000 times smaller than the diameter of a human hair – exhibit important changes for which traditional models and theories cannot explain. Developments in these emerging fields are likely to change the way almost everything – from vaccines to computers to automobile tires to objects not yet imagined – is designed and made.

The initiative will support long-term nanoscale research and development leading to potential breakthroughs in areas such as materials and manufacturing, nanoelectronics, medicine and healthcare, environment, energy, chemicals, biotechnology, agriculture, information technology, and national security. The effect of nanotechnology on the health, wealth, and lives of people could be at least as significant as the combined influences of microelectronics, medical imaging, computer-aided engineering, and man-made polymers developed in this century.

The initiative, which nearly doubles the nanoscale R&D investment over FY 2000, supports a broad range of scientific disciplines including material sciences, physics, chemistry, and biology, and creates new opportunities for interdisciplinary research. Agencies participating in the NNI include the National Science Foundation (NSF), the Department of Defense (DOD), the Department of Energy (DOE), National Institutes of Health (NIH), National Aeronautics and Space Administration (NASA), and the Department of Commerce's National Institute of Standards and Technology (DOC/NIST). Roughly 70% of the new funding proposed under the NNI will go to university-based research; funds that will help meet the growing demand for workers with nanoscale science and engineering skills. Nanoscience is still in its infancy and, outside of a handful of examples, only rudimentary nanostructures can be created with some control. It will take many years of sustained investment to achieve many of the NNI's research goals, but that is precisely why there is an important role for the Federal government.

Nanotechnology Research and Development Funding by Agency:

	FY 2000 ($M)	NNI ($M)	FY 2001 ($M)	Percent Increase
National Science Foundation	$97	$120	$217	124%
Department of Defense	$70	$40	$110	57%
Department of Energy	$58	$36	$94	66%
NASA	$5	$15	$20	300%
Department of Commerce	$8	$10	$18	125%
National Institutes of Health	$32	$4	$36	13%
TOTAL	$270	$225	$495	83%

The National Nanotechnology Initiative establishes **Grand Challenges** -- potential breakthroughs that if one day realized could provide major, broad-based economic benefits to the United States, as well as improve the quality of life for its citizens dramatically. Examples of these breakthroughs include:

- Containing the entire contents of the Library of Congress in a device the size of a sugar cube;
- Making materials and products from the bottom-up, that is, by building them up from atoms and molecules. Bottom-up manufacturing should require less material and create less pollution;
- Developing materials that are 10 times stronger than steel, but a fraction of the weight for making all kinds of land, sea, air and space vehicles lighter and more fuel efficient;
- Improving the computer speed and efficiency of minuscule transistors and memory chips by factors of millions making today's Pentium IIIs seem slow;
- Detecting cancerous tumors that are only a few cells in size using nanoengineered contrast agents;
- Removing the finest contaminants from water and air, promoting a cleaner environment and potable water at an affordable cost; and
- Doubling the energy efficiency of solar cells.

The NNI Investment Strategy:

The President's Committee of Advisors on Science and Technology (PCAST) strongly endorsed the establishment of the NNI, beginning in Fiscal Year 2001, saying that "now is the time to act." The PCAST noted the NNI as having "an excellent multi-agency framework to ensure U.S. leadership in this emerging field that will be essential for economic and national security leadership in the first half of the next century."

This initiative builds upon previous and current nanotechnology programs. The research strategy is balanced across five kinds of activities. In addition to the Grand Challenges discussed above, these activities include: fundamental research, centers and networks of excellence, research infrastructure, as well as ethical, legal and social implications and workforce programs:

- **Long-term fundamental nanoscience and engineering research** will build a fundamental understanding and lead to discoveries of the phenomena, processes, and tools necessary to control and manipulate matter at the nanoscale. This investment will provide sustained support to individual investigators and small groups doing fundamental research, promote university-industry-federal laboratory partnerships, and foster interagency collaborations.

- **Centers and Networks of Excellence** will encourage research networking and shared academic users' facilities. These nanotechnology research centers will play an important role in development and utilization of specific tools, and in promoting partnerships in the coming years.
- **Research Infrastructure** includes funding for metrology (measurement science), instrumentation, modeling and simulation, and user facilities. The goal is to develop a flexible and enabling infrastructure so that U.S. industry can rapidly commercialize the new discoveries and innovations.
- **Ethical, Legal, and Societal Implications, and Workforce Education and Training** efforts will promote a new generation of skilled workers with the multidisciplinary perspectives necessary for rapid progress in nanotechnology. Nanotechnology's effect on society -- legal, ethical, social, economic, and workforce preparation -- will be studied to help identify potential concerns and ways to address them.

Funding by NNI Research Portfolio:

	Fundamental Research	Grand Challenges	Centers And Networks of Excellence	Research Infrastructure	Ethical, Legal, and Social Implications and Workforce	Total
FY 2000	$87 M	$71 M	$47 M	$50 M	$15 M	$270 M
NNI	**$90 M**	**$62 M**	**$30 M**	**$30 M**	**$13 M**	**$225 M**
FY 2001	$177 M	$133 M	$77 M	$80 M	$28 M	$495 M

IMPLEMENTATION PLAN:

Funding of the recommended R&D priorities outlined above will be conducted by the participating agencies as a function of their mission and contingent on available resources. A coherent approach will be developed for funding the critical areas of nanoscience and engineering, establishing a balanced and flexible infrastructure, educating and training the necessary workforce, and promoting partnerships to ensure that these collective research activities provide a sound and balanced national research portfolio. By facilitating coordination and collaboration among agencies, the NNI will maximize the Federal government's investment in nanotechnology and avoid unnecessary duplication of efforts. The vision, strategy, agency participation, and agency partnerships for the five priorities are described in the full report.

Management:

The NNI will be managed within the framework of the National Science and Technology Council's (NSTC) Committee on Technology (CT). The Committee, composed of senior-level representatives from the Federal government's research and development departments and agencies, provides policy leadership and budget guidance for this and other multiagency technology programs.

The CT's Subcommittee on Nanoscale Science, Engineering, and Technology (NSET) will coordinate the Federal government's multiagency nanoscale R&D programs, including the NNI.

The NSET Subcommittee will coordinate planning, budgeting, implementing, and reviewing the NNI to ensure a broad and balanced initiative. The Subcommittee is composed of representatives from agencies with plans for future participation in the NNI and White House officials. The NSET Subcommittee is co-chaired by the White House National Economic Council (NEC) and a representative from an NNI participating agency as designated by the CT. Subcommittee representatives from agencies have operational authority over nanotechnology research and/or nanotechnology infrastructure within their own agency. The NSET Subcommittee succeeds the Interagency Working Group on Nanoscience, Engineering, and Technology (IWGN) as the primary interagency coordination mechanism. Currently, the NSET members are from DOC, DOD, DOE, Department of Transportation (DOT), Environmental Protection Agency (EPA), NASA, NIH, NSF, and White House offices (NEC, Office of Management and Budget (OMB), and Office of Science and Technology Policy (OSTP)).

Under the NNI, each agency will invest in those R&D projects that support its own mission as well as NNI goals. While each agency will consult with the NSET Subcommittee, the agency retains control over how it will allocate resources against its proposed NNI plan based on the availability of funding. Each agency will use its own methods for inviting and evaluating proposals. Each agency will evaluate its own NNI research activities according to its own Government Performance Review Act (GPRA) policies and procedures.

A National Nanotechnology Coordination Office (NNCO) will be established to serve as the secretariat to the NSET Subcommittee, providing day-to-day technical and administrative support. The NNCO will support the NSET Subcommittee in the preparation of multiagency planning, budget, and assessment documents. The NNCO will be the point of contact on Federal nanotechnology activities for government organizations, academia, industry, professional societies, foreign organizations, and others to exchange technical and programmatic information. In addition, the NNCO will develop and make available printed and other material as directed by the NSET Subcommittee, as well as maintain the NNI Web Site.

The NNCO Director will be an NSTC agency representative appointed by the Associate Director for Technology at the White House Office of Science and Technology Policy, in consultation with the Chair of the NSET Subcommittee and Executive Committee of the Committee on Technology. The NNCO Director reports to the Associate Director, but works in close collaboration with the Subcommittee Chair to establish goals and priorities for NNCO support**.** Agency detailees and contractors will staff the NNCO. The NNCO's annual funding will be derived from cash and in-kind contributions from agencies participating in the NNI, based on a percentage of each agency's total investment in nanoscale R&D. Beginning in FY 2002 and annually thereafter, the NNCO must submit a budget to the NSET Subcommittee for approval. If the NNCO's proposed budget is 15 percent or greater than the previous year, approval by the Executive Board of the Committee on Technology will be required.

The PCAST recommended in its letter to the President that a non-government advisory committee review the NNI annually to assess progress towards its goals. A report would be provided to the Committee on Technology. The Committee would work with the NSET Subcommittee to address issues raised by the outside advisory committee and to implement changes to the NNI strategy.

Initial discussions on such an advisory committee have been held between the members of the Committee on Technology and the National Research Council.

Coordination:

NNI coordination will be achieved though the NSET Subcommittee, direct interactions among program officers within the participating agencies, periodic management meetings and program reviews, and joint science and engineering workshops. The NSET Subcommittee will coordinate joint activities among agencies that create synergies or complement the individual agencies' activities to further NNI goals. Communication and collaborative activities are also facilitated by the NNI website (http://www.nano.gov) as well as by the agencies' sites dedicated to NNI.

Examples of NNI coordination include identification of the most promising research directions, encouraging funding of complementary fields of research across agencies that are critical for the advancement of the nanoscience and engineering field, education and training of the necessary workforce, and establishing a process by which centers and networks of excellence are selected.

The NNI coordination process began in 1999 with the preparation of the IWGN Research Directions. In the spring of 2000, NSET Subcommittee (formerly IWGN) members took part in planning activities at each agency. In addition, a survey is being conducted in all agencies participating in the NNI to identify opportunities for collaboration and areas where duplication can be avoided. Discussions are being held regarding joint exploratory workshops (such as those on molecular electronics, quantum computing, and nanobiotechnology) and agreements on specific interagency funding programs. Improved internal coordination in large agencies, concurrently with interagency collaboration, has also been noteworthy in the planning process.

Examples of major collaborative NNI activities planned by the participating agencies are:

Agency	**DOC**	**DOD**	**DOE**	**NASA**	**NIH**	**NSF**
Fundamental research		x	x	x	x	x
Nanostructured materials	x	x	x	x	x	x
Molecular electronics		x		x		x
Spin electronics		x		x		x
Lab-on-a-chip (nanocomponents)	x	x	x	x	x	x
Biosensors, bioinformatics				x	x	x
Bioengineering		x	x		x	x
Quantum computing	x	x	x	x		x
Measurements and standards for tools	x	x	x		x	x
Nanoscale theory, modeling, simulation		x	x	x		x
Environmental monitoring			x	x		x
Nanorobotics			x	x		x
Unmanned missions		x		x		
Nanofabrication user facilities	x		x	x	x	x

The NSET Subcommittee will reach out to the nanoscience and nanoengineering efforts of other nations. These emerging fields create a unique opportunity for the U.S. to partner with other countries in ways that are mutually beneficial. Potential activities include information sharing, cooperative research, and study by young U.S. scholars at foreign centers of excellence. In addition, the NSET Subcommittee will continue its worldwide survey study, DOD's international field offices will assess the nanoscience investment strategies and commercial interests in their geographies of responsibility.

Time line summary:

Below are the key deliverables in the next five years (Fiscal years 2001-2005). Out-year deliverables depend on regular increases in funding for this initiative.

Deliverable	***First Achieved***
Begin augmented research and development in fundamental research, grand challenges, infrastructure, education and nanotechnology societal impacts in response to open competitive solicitations and regular program reviews	FY 2001
Begin work on teams and centers for pursuing mission agency objectives	FY 2001
Establish ten new centers and networks with full range of nanoscale measurement and fabrication facilities	FY 2002
Develop new standard reference materials for semiconductor nanostructures, lab-on-a-chip-technologies, nanomagnetics, and calibration and quality assurance analysis for nanosystems	FY 2003
Develop standardized, reproducible, microfabricated approaches to nanocharacterization, nanomanipulation and nanodevices	FY 2004
Develop quantitative measurement methods for nanodevices, nanomanipulation, nanocharacterization and nanomagnetics; Develop 3-D measurement methods for the analysis of physical and chemical at or near atomic spatial resolution.	FY 2004
Ensure that 50 % of research institutions faculty and students have access to full range of nanoscale research facilities	FY 2005
Enable access to nanoscience and engineering education for students in at least 25% of research universities	FY 2005
Catalyze creation of several new commercial markets that depend on three-dimensional nanostructures	FY 2005
Develop three-dimensional modeling of nanostructures with increased speed/accuracy that allows practical system and architecture design	FY 2005

NATIONAL NANOTECHNOLOGY INITIATIVE –
LEADING TO THE NEXT INDUSTRIAL REVOLUTION

1. Initiative Overview

The "National Nanotechnology Initiative (NNI) – Leading to the Next Industrial Revolution" is part of the President's proposed fiscal year (FY) 2001 Federal budget. The initiative supports long-term nanoscale research and development leading to potential breakthroughs in areas such as materials and manufacturing, nanoelectronics, medicine and healthcare, environment and energy, chemical and pharmaceutical industries, biotechnology and agriculture, computation and information technology, and national security. The impact of nanotechnology on the health, wealth, and lives of people could be at least as significant as the combined influences of microelectronics, medical imaging, computer-aided engineering, and man-made polymers developed in this century. This new Federal investment will lead to a near doubling of the government's total investment in nanoscale R&D. The NNI incorporates fundamental research, Grand Challenges, centers and networks of excellence, and creating a research infrastructure – activities that are high risk, high payoff, and broadly enabling. This initiative also addresses development of novel approaches to the education and training of future nanotechnology workers, the ethical, legal and social implications of nanotechnology, and rapid transfer of knowledge and technology gained from the research and development efforts. The National Science and Technology Council Committee on Technology's Interagency Working Group on Nanoscience, Engineering and Technology (IWGN) prepared a few publications, as listed in Appendix C, that form the foundation for the evolution of the NNI.

In 1999, the President's Committee of Advisers on Science and Technology (PCAST) established a PCAST Nanotechnology Panel comprised of leading experts from academia and industry to provide a technical and budgetary review of the proposed NNI. Upon review, the PCAST strongly endorsed the establishment of the NNI, beginning in Fiscal Year 2001, saying that "now is the time to act." PCAST also noted the NNI has "an excellent multi-agency framework to ensure U.S. leadership in this emerging field that will be essential for economic and national security leadership in the first half of the next century." PCAST's endorsement to the President is attached in Appendix D.

The Administration is currently evaluating the mechanisms to establish a national nanotechnology coordination office that would support the NNI and an external review board of experts that would annually monitor the NNI goals.

2. Definition of Nanotechnology

The essence of nanotechnology is the ability to work at the molecular level, atom by atom, to create large structures with fundamentally new molecular organization. Compared to the behavior of isolated molecules of about 1 nm (10^{-9} m) or of bulk materials, behavior of structural features in the range of about 10^{-9} to 10^{-7} m (1 to 100 nm - a typical dimension of 10 nm is 1,000 times smaller than the diameter of a human hair) exhibit important changes. Nanotechnology is concerned with materials and systems whose structures and components exhibit novel and significantly improved

physical, chemical, and biological properties, phenomena, and processes due to their nanoscale size. The goal is to exploit these properties by gaining control of structures and devices at atomic, molecular, and supramolecular levels and to learn to efficiently manufacture and use these devices. Maintaining the stability of interfaces and the integration of these "nanostructures" at micron-length and macroscopic scales are all keys to success.

New behavior at the nanoscale is not necessarily predictable from that observed at large size scales. The most important changes in behavior are caused not by the order of magnitude size reduction, but by newly observed phenomena intrinsic to or becoming predominant at the nanoscale. These phenomena include size confinement, predominance of interfacial phenomena and quantum mechanics. Once it becomes possible to control feature size, it will also become possible to enhance material properties and device functions beyond what we currently know how to do or even consider as feasible. Being able to reduce the dimensions of structures down to the nanoscale leads to the unique properties of carbon nanotubes, quantum wires and dots, thin films, DNA-based structures, and laser emitters. Such new forms of materials and devices herald a revolutionary age for science and technology, provided we can discover and fully utilize the underlying principles.

3. A Revolution in the Making: Driving Forces

In 1959 Richard Feynman delivered his now famous lecture, "There is Plenty of Room at the Bottom." He stimulated his audience with the vision of exciting new discoveries if one could fabricate materials and devices at the atomic/molecular scale. He pointed out that, for this to happen, a new class of miniaturized instrumentation would be needed to manipulate and measure the properties of these small—"nano"—structures.

It was not until the 1980s that instruments were invented with the capabilities Feynman envisioned. These instruments, including scanning tunneling microscopes, atomic force microscopes, and near-field microscopes, provide the "eyes" and "fingers" required for nanostructure measurement and manipulation. In parallel, the expansion of computational capability enabled sophisticated simulations of material behavior at the nanoscale. These new tools and techniques have sparked excitement throughout the scientific community. Traditional models and theories for material properties and device operations involve assumptions based on "critical scale lengths" that are generally larger than 100 nanometers. When at least one dimension of a material structure is under this critical length, distinct behavior often emerges that cannot be explained by traditional models and theories. Thus, scientists from many disciplines are avidly fabricating and analyzing nanostructures to discover novel phenomena at the intermediate scale between individual atoms/molecules and hundred of thousand of molecules where the novel phenomena develop. Nanostructures offer a new paradigm for materials manufacture by utilizing submicron-scale assembly to create entities from the "bottom up" rather than the "top down" ultraminiaturization method of chiseling smaller structures from larger ones. However, researchers are just beginning to understand some of the principles to use to create "by design" nanostructures and how to economically fabricate nanodevices and systems. Even when fabricated, though, the physical and chemical properties of those nanostructured devices are just beginning to be uncovered. Models developed for micron-size and larger devices only work at scale lengths greater than the 100+ nm range. Each significant advance in understanding the physical, chemical, and biological properties

of nanostructures, and in the development of principles and predictive methods to fabricate and control them, will increase researchers' ability to design, fabricate and assemble the nanostructures and nanodevices into a working system.

Federal support of the nanotechnology is necessary to enable the United States to take advantage of this strategic technology and remain competitive in the global marketplace well into the future. Focused research programs on nanotechnology have been initiated in almost all industrialized countries in the last five years. Currently, the United States has a lead on synthesis, chemicals, and biological aspects; it lags in research on nanodevices, production of nano-instruments, ultra-precision engineering, ceramics, and other structural materials. Japan has an advantage in nanodevices and consolidated nanostructures; Europe is strong in dispersions, coatings, and new instrumentation. Japan, Germany, U.K., Sweden, Switzerland, and EU all are creating centers of excellence in specific areas of nanotechnology.

4. Nanotechnology's Impact

The potential benefits of nanotechnology are pervasive, as illustrated in the fields outlined below:

Materials and Manufacturing. Nanotechnology is fundamentally changing the way materials and devices will be produced in the future. The ability to synthesize nanoscale building blocks with precisely controlled size and composition and then to assemble them into larger structures with unique properties and functions will revolutionize segments of the materials manufacturing industry. Some of the benefits that nanostructuring can bring include lighter, stronger, and programmable materials; reductions in life-cycle costs through lower failure rates; innovative devices based on new principles and architectures; and use of molecular/cluster manufacturing, which takes advantage of assembly at the nanoscale level for a given purpose. Researchers will be able to develop structures not previously observed in nature. Challenges include synthesis of materials by design, development of bio- and bio-inspired materials, development of cost-effective and scalable production techniques, and determination of the nanoscale initiators of materials failure. Applications include (a) manufacturing of nanostructured metals, ceramics and polymers at exact shapes without machining; (b) improved printing brought about by nanometer-scale particles that have the best properties of both dyes and pigments; (c) nanoscale cemented and plated carbides and nanocoatings for cutting tools, electronic, chemical, and structural applications; (d) new standards for measurements at nanoscale, and (d) nanofabrication on a chip with high levels of complexity and functionality.

Nanoelectronics and Computer Technology. The Semiconductor Industry Association (SIA) has developed a roadmap for continued improvements in miniaturization, speed, and power reduction in information processing devices—sensors for signal acquisition, logic devices for processing, storage devices for memory, displays for visualization, and transmission devices for communication. The SIA roadmap projects the future to approximately 2010 and to 0.1-micron (100 nm) structures, just short of fully nanostructured devices. The roadmap ends just short of true nanostructure devices because the principles, fabrication methods, and the way to integrate devices into systems are generally unknown. The SIA roadmap explicitly calls for "sustained government support if this industry is to continue to provide for strong economic growth in the U.S." The lead

time for science maturing into technology is approximately 10 to 15 years; now is the critical time for government investment in the science and technology of nanostructures for the hardware necessary to satisfy continuing demands in information technology. Further, the investment will have spin-offs that enable the attainment (or acceleration) of other SIA roadmap goals. The area of magnetic information storage is illustrative. Within ten years of the fundamental discovery of the new phenomenon of giant magnetoresistance, this nanotechnology completely replaced older technologies for disk computer heads, leveraging a market worth $34 billion in 1998. Other potential breakthroughs include (a) nanostructured microprocessor devices that continue the trend in lower energy use and cost per gate, thereby improving the efficacy of computers by a factor of millions; (b) communications systems with higher transmission frequencies and more efficient utilization of the optical spectrum to provide at least ten times more bandwidth, with consequences in business, education, entertainment, and defense; (c) small mass storage devices with capacities at multi-terabit levels, a thousand times better than today; and (d) integrated nanosensor systems capable of collecting, processing, and communicating massive amounts of data with minimal size, weight, and power consumption. Potential applications of nanoelectronics also include affordable virtual reality stations that provide individualized teaching aids (and entertainment); computational capability sufficient to enable unmanned combat and civilian vehicles; and communication capability that obviates much commuting and other business travel in an era of increasingly expensive transport fuels.

Medicine and Health. Living systems are governed by molecular behavior at nanometer scales where the disciplines of chemistry, physics, biology, and computer simulation all now converge. Such multidisciplinary insights will stimulate progress in nanobiotechnology. The molecular building blocks of life—proteins, nucleic acids, lipids, carbohydrates and their non-biological mimics—are examples of materials that possess unique properties determined by their size, folding, and patterns at the nanoscale. Recent insights into the uses of nanofabricated devices and systems suggest that today’s laborious process of genome sequencing and detecting the genes’ expression can be made dramatically more efficient through utilization of nanofabricated surfaces and devices. Expanding our ability to characterize an individual’s genetic makeup will revolutionize the specificity of diagnostics and therapeutics. Beyond facilitating optimal drug usage, nanotechnology can provide new formulations and routes for drug delivery, enormously broadening their therapeutic potential. Increasing nanotechnological capabilities will also markedly benefit basic studies of cell biology and pathology. As a result of the development of new analytical tools capable of probing the world of the nanometer, it is becoming increasingly possible to characterize the chemical and mechanical properties of cells (including processes such as cell division and locomotion) and to measure properties of single molecules. These capabilities thus complement (and largely supplant) the ensemble average techniques presently used in the life sciences. Moreover, biocompatible, high-performance materials will result from controlling their nanostructure. Proteins, nucleic acids, and lipids, or their nonbiological mimics, are example of materials that have been shown to possess unique properties as a function of their size, folding, and patterns. Based on these biological principles, bio-inspired nanosystems and materials are currently being formed by self-assembly or other patterning methods. Artificial inorganic and organic nanoscale materials can be introduced into cells to play roles in diagnostics (e.g., quantum dots in visualization), but also potentially as active components. Finally, nanotechnology-enabled increases in computational power will permit the characterization of macromolecular networks in realistic environments. Such simulations will be essential in developing biocompatible implants and in the drug discovery process. Potential

applications include (a) rapid, more efficient genome sequencing enabling a revolution in diagnostics and therapeutics; (b) effective and less expensive health care using remote and in-vivo devices; (c) new formulations and routes for drug delivery that enormously broaden their therapeutic potential by targeting the delivery of new types of medicine to previously inaccessible sites in the body; (d) more durable rejection-resistant artificial tissues and organs; (e) enable vision and hearing aids; and (f) sensor systems that detect emerging disease in the body, which will ultimately shift the focus of patient care from disease treatment to early detection and prevention.

Aeronautics and Space Exploration. The stringent fuel constraints for lifting payloads into earth orbit and beyond, and the desire to send spacecraft away from the sun (diminished solar power) for extended missions, compel continued reduction in size, weight, and power consumption of payloads. Nanostructured materials and devices promise solutions to these challenges. Nanostructuring is also critical to design and manufacture of lightweight, high-strength, thermally stable materials for planes, rockets, space stations, and planetary/solar exploratory platforms. Moreover, the low-gravity, high-vacuum space environment may aid development of nanostructures and nanoscale systems that cannot be created on Earth. Applications include (a) low-power, radiation-tolerant, high performance computers; (b) nano-instrumentation for microspacecraft; (c) avionics made possible by nanostructured sensors and nanoelectronics; and (d) thermal barrier and wear-resistant nanostructured coatings.

Environment and Energy. Nanotechnology has the potential to significantly impact energy efficiency, storage, and production. It can be used to monitor and remediate environmental problems; curb emissions from a wide range of sources; and develop new, "green" processing technologies that minimize the generation of undesirable by-product effluents. The impact on industrial control, manufacturing, and processing will be impressive and result in energy savings through market driven practices. Several new technologies that utilize the power of nanostructuring but developed without benefit of the new nanoscale analytical capabilities, illustrate this potential: (a) a long-term research program in the chemical industry into the use of crystalline materials as catalyst supports has yielded catalysts with well-defined pore sizes in the range of 1 nm; their use is now the basis of an industry that exceeds $30 billion/year; (b) the discovery of the ordered mesoporous material MCM-41 produced by oil industry, with pore sizes in the range of 10-100 nm, is now widely applied in removal of ultrafine contaminants; (c) several chemical manufacturing companies are developing a nanoparticle-reinforced polymeric material that can replace structural metallic components in the auto industry; widespread use of those nanocomposites could lead to a reduction of 1.5 billion liters of gasoline consumption over the life of one year's production of vehicles and reduce related carbon dioxide emissions annually by more than 5 billion kilograms; and (d) the replacement of carbon black in tires by nanometer-scale particles of inorganic clays and polymers is a new technology that is leading to the production of environmentally friendly, wear-resistant tires. Potential future breakthroughs also include use of nanorobotics and intelligent systems for environmental and nuclear waste management, use of nanofilters to separate isotopes in nuclear fuel processing, of nanofluids for increased cooling efficiency of nuclear reactors, of nanopowders for decontamination, and of computer simulation at nanoscale for nuclear safety.

Biotechnology and Agriculture. The molecular building blocks of life - proteins, nucleic acids, lipids, carbohydrates and their non-biological mimics - are examples of materials that possess unique properties determined by their size, folding and patterns at the nanoscale. Biosynthesis and

bioprocessing offer fundamentally new ways to manufacture new chemicals and pharmaceutical products. Integration of biological building blocks into synthetic materials and devices will allow the combination of biological functions with other desirable materials properties. Imitation of biological systems provides a major area of research in several disciplines. For example, the active area of bio-mimetic chemistry is based on this approach. Nanoscience will contribute directly to advancements in agriculture in a number of ways: molecular-engineered biodegradable chemicals for nourishing the plants and protecting against insects; genetic improvement for animals and plants; delivery of genes and drugs to animals; and nanoarray-based testing technologies for DNA testing. For example, such array-base technologies will allow a plant scientist to know which genes are expressed in a plant when its is exposed to salt or drought stress. The application of nanotechnology in agriculture has only begun to be appreciated.

National Security. The Department of Defense recognized the importance of nanostructures over a decade ago and has played a significant role in nurturing the field. Critical defense applications include (a) continued information dominance through advanced nanoelectronics, identified as an important capability for the military; (b) more sophisticated virtual reality systems based on nanostructured electronics that enable more affordable, effective training; (c) increased use of enhanced automation and robotics to offset reductions in military manpower, reduce risks to troops, and improve vehicle performance; for example, several thousand pounds could be stripped from a pilotless fighter aircraft, resulting in longer missions, and fighter agility could be dramatically improved without the necessity to limit g-forces on the pilot, thus increasing combat effectiveness; (d) achievement of the higher performance (lighter weight, higher strength) needed in military platforms while simultaneously providing diminished failure rates and lower life-cycle costs; (e) badly needed improvements in chemical/biological/nuclear sensing and in casualty care; (f) design improvements of systems used for nuclear non-proliferation monitoring and management; and (g) combined nano and micromechanical devices for control of nuclear defense systems.

Other Potential Government Applications. Nanoscience and technology can benefit other Government agency missions, including (a) lighter and safer equipment in transportation systems; (b) measurement, control, and remediation of contaminants; (c) enhanced forensic research (Department of Justice, DOJ); and (d) printing and engraving of high quality, forgery-proof documents and currency (Bureau of Engraving and Printing, BEP).

Science and Education. Advances in nanoscale science, engineering, and technology will require and enable advances in many disciplines: physics, chemistry, biology, materials, mathematics, and engineering. The dynamics of these interdisciplinary nanoscale research efforts will reinforce educational connections among disciplines and give birth to new fields that are only envisioned at this moment. The interdisciplinary nature of nanoscale science, engineering, and technology requires changes in how students and professional are educated and trained for careers in these fields.

Future U.S. Competitiveness. Technology is the major driving factor for growth at every level of the U.S. economy. Nanotechnology is expected to be pervasive in its applications across nearly all technologies. Investment in nanotechnology research and development is necessary to maintain and improve our position in the world marketplace. A national nanotechnology initiative will allow the development of critical enabling technologies with broad commercial potential, such as

nanoelectronics, nanostructured materials and nanoscale-based manufacturing processes. These are necessary for U.S. industry to take advantage of nanotechnology innovations.

5. Investment Opportunities

Need for Investment. Nanoscale scientific, engineering, and technical knowledge is exploding worldwide. It is being made possible by the availability of new investigative tools, synergies created through an interdisciplinary approach, rapid dissemination of results, and driven by emerging technologies and their applications. With sustained investment, the number of revolutionary discoveries reported in nanotechnology can be expected to accelerate in the next decade; these are likely to profoundly affect existing and emerging technologies in almost all industry sectors and application areas. Over the past few years, it has become evident that there is a clear need for Federal support to create a balanced infrastructure for nanoscale science, engineering, technology and human resources development, and to address critical areas of research. The field is highly competitive and dynamic on international arena. The time now appears right for the nation to establish a significant R&D initiative to support nanotechnology.

Federal Government expenditure for nanotechnology in FY 1997 was approximately $116 million, according to the 1998 WTEC report "*R&D Status and Trends in Nanoparticles, Nanostructured Materials, and Nanodevices in the United States*" (NTIS Report PB98-117914). Nanotechnology as defined there only included work to generate and use nanostructures and nanodevices; it did not include the simple observation and description of phenomena at the nanoscale. Utilizing the broader definition, the Federal Government expenditure is estimated to be about $270 million for FY 2000. A much greater investment could be utilized effectively. There are signs of a significant increase in interest within the research community. For example, the funding success rate for the small-group interdisciplinary research program, FY 1998 NSF "Functional Nanostructures" initiative, was about 13% (lower, if one considers the limitation of two proposals per university). The success rate for the DOD 1998 MURI initiative on nanostructures was 17% (5%, if one starts with the number of white papers submitted to guide proposal development). In both instances, the level of funding available limited the funding success rate. There were more meritorious proposals than could be supported at that time.

The promises of nanotechnology can best be realized through long term and balanced investment in U.S. infrastructure and human resources in five R&D categories in particular: (1) Nanostructure *properties*: Develop and extend our understanding of biological, chemical, materials science, electronic, magnetic, optical, and structural properties in nanostructures; (2) Synthesis *and processing*: Enable the atomic and molecular control of material building blocks and develop engineering tools to provide the means to assemble and utilize these tailored building blocks for new processes and devices in a wide variety of applications. Extend the traditional approaches to patterning and microfabrication to include parallel processing with proximal probes, self-assembling, stamping, and templating. Pay particular attention to the interface with bionanostructures and bio-inspired structures, multifunctional and adaptive nanostructures, scaling approaches, and commercial affordability; (3) Characterization *and manipulation*: Discover and develop new experimental tools to broaden the capability to measure and control nanostructured matter, including developing new standards of measurement. Pay particular attention to tools

capable of measuring/manipulating single macro- and supra-molecules of biological interest; (4) Modeling *and simulation*: Accelerate the application of novel concepts and high-performance computation to the prediction of nanostructured properties, phenomena, and processes; (5) Device *and system concepts*: Stimulate the innovative application of nanostructure properties in ways that might be exploited in new technologies.

International Perspective. The United States does not dominate nanotechnology research. There is strong international interest, with nearly twice as much ongoing research overseas as in the United States (see the worldwide study *Nanostructure Science and Engineering*, NSTC 1999). Other regions, particularly Japan and Western Europe, are supporting work that is equal to the quality and breadth of the science done in the United States because there, too, scientists and national leaders have determined that nanotechnology has the potential to be a major economic factor during the next several decades. This situation is unlike the other post-war technological revolutions, where the United States enjoyed earlier leads. The international dimensions of nanotechnology research and its potential applications implies that the United States must put in place an infrastructure that is equal to that which exists anywhere in the world. This emerging field also creates a unique opportunity for the United States to partner with other countries in ways that are mutually beneficial through information sharing, cooperative research, and study by young U.S. researchers at foreign centers of excellence. A suitable U.S. infrastructure is also needed to compete and collaborate with those groups.

6. High-Level Recognition of Nanotechnology's Potential

The promise of nanoscience and engineering has not passed unnoticed. Dr. Neal Lane, currently the President's Advisor for Science and Technology and former NSF director, stated at a Congressional hearing in April 1998, "If I were asked for an area of science and engineering that will most likely produce the breakthroughs of tomorrow, I would point to nanoscale science and engineering." In March 1998, Dr. John H. Gibbons, Dr. Lane's predecessor, identified nanotechnology as one of the five technologies that will determine economic development in the next century. Several federal agencies have been actively investigating nanoscience R&D. NSF started the Nanoparticle Synthesis and Processing initiative in 1991 and the National Nanofabrication User Network in 1994, and has highlighted nanoscale science and engineering in its FY 1998 budget. The Defense Department identified nanotechnology as a strategic research objective in 1997. NIH identified nanobiotechnology as a topic of interest in its 1999 Bioengineering Consortium (BECON) program.

More recently, on May 12, 1999, Richard Smalley, Nobel Laureate, concluded in his testimony to the Senate Subcommittee on Science, Technology, and Space that "We are about to be able to build things that work on the smallest possible length scales. It is in our Nation's best interest to move boldly into this new field." On June 22, 1999, the Subcommittee on Basic Research of the Committee on Science organized the hearing on "Nanotechnology: The State of Nano-Science and Its Prospects for the Next Decade". The Subcommittee Chairman Nick Smith, of Michigan concluded the hearings stating that "Nanotechnology holds promise for breakthroughs in health, manufacturing, agriculture, energy use and national security. It is sufficient information to aggressively address funding of this field."

7. Proposed Federal Contribution to the NNI

Government's role in nanoscience and technology. While nanotechnology research is in an early stage, it already has several promising results. It is clear that it can have a substantial impact on industry and on our standard of living by improving healthcare, environment and economy. But investments must be made in science and engineering that will enable scientists and engineers to invent totally new technologies and enable industry to produce cost-competitive products. Since many of the findings on nanostructures and nanoprocesses are not yet fully measurable, replicable, or understood, it will take many years to develop corresponding technologies. Industry needs to know what are the principles of operation and how to economically fabricate, operate, and integrate nanostructured materials and devices. Private industry is unable in the usual 3-5 year industrial product time frame to effectively develop cost-competitive products based on current knowledge. Further, the necessary fundamental nanotechnology research and development is too broad, complex, expensive, long-term, and risky for industry to undertake. Thus, industry is not able to fund or is significantly under-funding critical areas of long-term fundamental research and development and is not building a balanced nanoscience infrastructure needed to realize nanotechnology's potential.

Thus far, Federal and academic investments in nanoscale science, engineering, and technology have occurred in open competition with other research topics within various disciplines. This dynamics is one reason that U.S. nanotechnology research efforts tend to be fragmented and overlap among disciplines, areas of relevance, and sources of funding. It is important to develop a strategic research and development and implementation plan. A coordinated national effort could focus resources on stimulating cooperation, avoid unwanted duplication of efforts, capture the imagination of young people, and support of basic sciences. The government should support expansion of university and government laboratory facilities, help to build the workforce skills necessary to staff future industries based on nanotechnology and future academic institutions, encourage cross-disciplinary networks and partnerships, ensure the dissemination of information, and encourage small businesses to exploit the nanotechnology opportunities.

Nanotechnology R&D require long-term Federal investment. Nano- science and engineering R&D will need a long-term investment commitment because of their interdisciplinary characteristics, the limitations of the existing experimental and modeling tools in the intermediate range between individual molecules and microstructure, and the need for technological infrastructure. The time from fundamental discovery to market is typically 10-15 years (see for instance the application of magnetoresistance, and of mesoporous silicate for environmental and chemical industry applications). Historically, industry becomes a major player only in the last 3-5 years, when their investments are much larger than in the previous period, but the economic return is more certain. Industry is frequently reluctant to invest in risky research that takes many years to develop into a product. In the United States, the government and university research system can effectively fill this niche.

Government leadership and funds are needed to help implement policies and establish the nanotechnology infrastructure and research support in the next decade. Since major industrial markets are not yet established for nanotechnology products, it is proposed that the government support technology transfer activities to private industry to accelerate the long-term benefits. The

enabling infrastructure and technologies must be in place for industry to take advantage of nanotechnology innovations and discoveries. The increasing pace of technological commercialization requires a compression of past time scales, parallel development of research and commercial products, and a synergy among industry, university, and government partners. The government role will be on crosscutting, long-term research and development nanotechnology areas identified in this report.

Budget summaries for participating departments and agencies are as follows:

- **Current level of support**: The estimated nanotechnology funding in FY 1999 is approximately $255 million, and for FY 2000 is $270 million.
- **The proposed investments in FY 2001:** The total proposed increase in Federal expenditures for all participating departments and agencies for FY 2001 is $225 million. Table I illustrates the Federal agency investments from 1999 onward.

Table I. National Nanotechnology Initiative funding (in $ millions)

Agency	FY 1999 ($ M)	FY 2000 ($ M)	FY 2001 (+from FY 2000) ($ M)	Percentage Increase (%)
DOC/NIST	16 (with ATP)	8	18 (+10)	125%
DOD	70	70	110 (+40)	57%
DOE	58	58	94 (+36)	62%
NASA	5	5	20 (+15)	300%
NIH	21	32	36 (+4)	13%
NSF	85	97	217 (+120)	124%
Total	255	270	495 (+225)	83%

Funding themes and modes of research proposed for Funding Agencies in FY 2001: Below is an outline of the funding mechanisms (for more details on specific plans for each theme – please see Appendices A1 to A5).

1. <u>Fundamental research (total FY 2001 is $177 million, $90 million above FY 2000)</u>. Fund single investigators and small groups with awards of $200-500K each. This investment will provide sustained support to individual investigators and small groups conducting fundamental, innovative research; larger investment should be given at the beginning to funding fundamental research, as well as to development of university-industry-laboratory and interagency partnerships.

2. <u>Grand Challenges (total FY 2001 is $133 million, $62 million above FY 2000)</u>. Fund interdisciplinary research and education teams, that aim to achieve major, long-term objectives, as outlined below:
   a. *Nanomaterials 'by design' –stronger, lighter, harder, self-repairing and safer*: Structural carbon and ceramic materials ten times stronger than steel for use in industry, transportation,

and construction; polymeric materials three times stronger than present materials, melting at 100°C higher temperature, for use in cars and appliances; and "smart" multifunctional materials;

b. *Nano-electronics, optoelectronics and magnetics*: Nanometer structures for minuscule transistors and memory chips that will improve the computer speed and efficiency by factors of millions; expansion of mass storage electronics to multi-terabit memory capacity that will increase the memory storage per unit surface a thousand fold and make data available on a pinhead; changes in communication paradigms by increasing bandwidth a hundred times, which will reduce business travel and commuting;

c. *Healthcare*: Effective and less expensive health care by remote and in-vivo diagnostics and treatment devices; diagnostics and therapeutics using rapid genome sequencing and intracellular sensors; gene and drug delivery to targeted cancer cells and organs in the human body; earlier detection of cancer by nanoengineered MRI contrast agents; biosensors that will allow earlier detection of diseases, 50 percent reduction in rejection rate of artificial organs; and use of tiny medical devices that will minimize collateral damage of human tissues;

d. *Nanoscale processes and environment*: Removal of the finest contaminants from water (under 300 nm) and air (under 50 nm), and continuous measurement in large areas of the environment; Water purification and desalinization desalting seawater with at least 10 times less energy that state-of–the art reverse osmosis.

e. *Energy*: Dramatic improvement in the efficiency of energy conversion and storage; double the efficiency of solar cells;

f. *Microspacecraft*: Continuous presence in space outside of the solar system with low-powered microspacecraft;

g. *Bio-nanodevices for detection and mitigation of threats to humans*: Efficient and rapid bio-chemical detection and mitigation in situ for chemical-biowarfare, HIV, and tuberculosis; Miniaturized electrical/mechanical/chemical devices will extend human performance, protect health, and repair cellular/tissue damage; The research into these basic devices will be coordinated with the Healthcare Grand Challenges;

h. *Economical and safe transportation*: Adoption of novel materials, electronics, energy, and environmental concepts;

i. *National security*: *Maintain* defense superiority, with special attention to the nanoelectronics, multifunctional materials and bionanodevices Grand Challenges.

3. <u>Centers and networks of excellence (total FY 2001 is $77 million, $30 million above FY 2000)</u>. Fund ten new centers at about $3 million each for five years with opportunity of one renewal after the review. Encourage research networking and shared academic users' facilities. Establish nanotechnology research centers similar to supercomputer centers that will play an important role in reaching other initiative priorities (fundamental research, Grand Challenges and education), in development and utilization of the specific tools, and in promoting partnerships in the next decade.

4. <u>Research infrastructure (total FY 2001 is $80 million, $30 million above FY 2000)</u>. Increase funding for metrology ($7 million), instrumentation ($8 million), modeling and simulation ($6 million), and user facilities ($9 million). Encourage university-industry-national laboratory and international collaborations as well as knowledge and technology transfer between universities

and industry. Develop a flexible enabling infrastructure so that new discoveries and innovations can be rapidly commercialized by U.S. industry.

5. Societal implications of nanotechnology and workforce education and training (total $28 million, $13 million above FY 2000). Fund student fellowships/traineeships and curriculum development on nanotechnology; and change the general teaching paradigms with new teaching tools. Focused research on societal implications of nanotechnology, including social, ethical, legal, economic and workforce implications will be undertaken.

Priority research areas for increases in nanotechnology funding in FY 2001 over FY 2000:

A. *Long-term fundamental nanoscience and engineering research*. The goal is to build a fundamental understanding and to discover novel phenomena, processes, and tools for nanotechnology. Tools refer to measurement, modeling, simulation, and manipulation. This commitment will lead to potential breakthroughs and accelerated development in areas such as medicine and healthcare, materials and advanced manufacturing, computer technology, environment and energy. Early and focused government investments led to the success of today's computer technology and biotechnology industries. The NNI looks to focus the Government's investment on nanotechnology in a similar manner and with similar results.
B. *Synthesis and processing "by design"* of engineered, nanometer-size, material building blocks and system components, fully exploiting molecular self-organization concepts. This commitment will generate new classes of high-performance materials and bio-inspired systems; changes in device design paradigms; and efficient, affordable manufacturing of high-performance products. Novel properties and phenomena will be enabled as control of structures of atoms, molecules, and clusters become possible.
C. *Research in nanodevice concepts and system architecture*. The goal is to exploit properties of new nanodevice principles in operational systems and combine building-up of molecular structures with ultra-miniaturization. Nanodevices will cause fundamental changes such as orders-of-magnitude improvements in microprocessors and mass storage, widespread use of selective drug and gene delivery systems, tiny medical tools that minimize collateral human tissue damage, and unmanned combat vehicles in fully imaged battlefields. There will be dramatic payback to other programs with National priority in fields such as information technology, nanobiotechnology, and medical technology.
D. *Application of nanostructured materials and systems* to manufacturing, power systems, energy, environment, national security, and health care. Research is needed in advanced dispersions, catalysts, separation methods, and consolidated nanostructures. Also needed is development of core enabling technologies such as fundamental molecular scale measurement and manipulation tools and standard methods, materials, and data that can be applied to many commercial sectors.
E. *Education and training* of a new generation of skilled workers in the multidisciplinary perspectives necessary for rapid progress in nanotechnology. Study the impact of nanotechnology on the society at large, including economic, social, ethical and legal considerations.

Table II illustrates the NNI research portfolio by themes in FY 2001, as well as the FY 2001 increment above FY 2000 by each agency.

Table II. Funding by NNI Research Portfolio in FY 2001
The data in parenthesis are FY 2001 increments above FY 2000. All budgets are in $ millions.
(Note the estimations for individual themes may change depending on the merit review process)

Agency	Fundamental Research	Grand Challenges	Centers and Networks of Excellence	Research Infrastructure	Societal Implications and Workforce	Total
DOC/NIST		10 (+5)		6 (+4)	2 (+1)	18 (+10)
DOD	10 (+4)	54 (+23)	24 (+8)	19 (+5)	3 (+0)	110 (+40)
DOE	34 (+17)	29 (+16)	15 (+0)	16 (+3)		94 (+36)
NASA	4 (+3)	11 (+8)		5 (+4)		20 (+15)
NIH	7 (+1)	17 (+1)	1 (+1)	9 (+1)	2 (+0)	36 (+4)
NSF	122 (+65)	12 (+9)	37 (+21)	25 (+13)	21 (+12)	217 (+120)
Total	177 (+90)	133 (+62)	77 (+30)	80 (+30)	28 (+13)	495 (+225)

Individual Agencies' Activities in the Initiative. A preliminary inventory of activities is outlined below. The participating agencies are DOC, DOD, DOE, NASA, NIH, and NSF. Other agencies with nanotechnology-related activities included in other programs may be added in the future such as DOJ (with interest in forensic research, high performance computing, and data base management), DOT (with interest in advanced concepts for transportation security and nanostructured materials and sensors for physical transportation infrastructure), EPA (with interest in measurement and remediation of nanoparticles in air, water, and soil), and the Treasury Department (with interest in special colloidal suspensions at BEP). The following topics are addressed for each of the participating agencies (Note that all dollar figures are estimates that may change depending on the merit review process):

Department of Commerce (DOC, NIST, TA)

a. Total FY 2001 request is $18 million, $10 million above FY 2000. Requested increase is for measurement, standards, and economic and foreign assessment studies.
b. Major interests in nanotechnology: measurement science and standards, including methods, materials, and data; development and acceleration of enabling commercial technologies through industry-led joint ventures.
c. Estimated funding in FY 1999: $8.4 million for measurement and standards research, and approximately $8 million in FY 1998 Advanced Technology Program (ATP) cost-shared awards to U.S. industry in FY 1998; Estimated funding in FY 2000: $8.4 million for measurement and standards research.
d. Modes of R&D support: Development of measurement and standards infrastructure to support U.S. industry development and commercialization of nanotechnology; conduct of economic and foreign assessment studies.
e. Major themes and new programs in FY 2001 include
    - Nanodevices and biotechnology for quantum level measurement and calibration (corresponds to the priority research areas A, B, C, D listed on page 30)
    - Magnetic measurements and standards research (priorities A, C, D)
    - Nanoscale characterization: measurement systems, approaches and algorithms; standard data and materials (priorities A, C, D)

- Nanoscale manipulation for synthesis and fabrication of measurement systems and standards (priorities A, B, D)
- Study the economic, social and legal aspects (priority E)

Department of Defense (DOD)

a. Total FY 2001 request is $110 million, $40 million over FY 2000.
b. Major interests in nanotechnology: Information acquisition, processing, storage and display; materials performance and affordability; chemical and biological warfare defense.
c. Estimated funding in FY 1999 and FY 2000: $70 million in mainstream nanotechnology. The main topics are: novel phenomena, processes, and tools for characterization and manipulation ($19 million); nanoelectronics ($40 million), bio-chemical sensing ($1 million), and materials ($10 million).
d. Modes of R&D support: Principally university-based programs for individual investigators ($22 million) and centers ($8 million), some programs at the DOD laboratories ($5 million); and infrastructure (equipment, high performance computing, $5 million).
e. Major themes and new programs in FY 2001 include:
    - Advanced processes and tools (priority research areas A to D listed on page 30)
    - Nanostructured materials and systems(priority C)
    - Multifunctional electronics and materials "by design" (priorities A to D)
    - University centers focused on nanotechnology (priorities A-E)

Department of Energy (DOE)

a. Total FY 2001 request is $94 million, $36 million over FY 2000. Requested increment increase in FY 2001 is for $34 million for fundamental research, $29 million for Grand Challenges, $15 million for centers, and $16 million for research infrastructure.
b. Major interests in nanotechnology: Basic energy science and engineering, with research relevant to energy efficiency, defense, environment, and nuclear nonproliferation.
a. Estimated funding in FY 1999 and FY 2000: Approximately $58 million ($35 million materials, $11 million chemistry; $7 million defense, $1 million engineering).
b. Modes of R&D support: Capital development at national labs; secondary funding of universities for collaboration with DOE labs; support of national labs to work with other government agencies and industry; 2-3 laboratory user facilities.
c. Major themes and new programs in FY 2001 include
    - Research user facilities at four national laboratories, with a different focus (priority research areas A to E listed on page 30)
    - Academic support for energy and environment related topics (priorities A, B, D, E)

National Aeronautics and Space Agency (NASA)

a. Total FY 2001 request is $20 million, $15 million above FY 2000.
b. Major interests in nanotechnology: Lighter and smaller spacecraft, biomedical sensors and medical devices, powerful computers that are smaller and consume less power, radiation-tolerant electronics, thin film materials for solar sails.
c. Estimated funding: $5.3 million in FY 1999 (additional $13 million are spent in other targeted programs), and $5 million in FY 2000.
d. Modes of R&D support: Fund NASA laboratory research and academic research.

e. Major themes and new programs in FY 2001 include: – Manufacturing techniques of single walled carbon nanotubes for structural reinforcement; electronic, magnetic, lubricating, and optical devices; chemical sensors and biosensors (priority research areas B, C, D listed on page 30)
   - Tools to develop autonomous devices that articulate, sense, communicate, and function as a network, extending human presence beyond the normal senses (priorities C, D)
   - Robotics using nanoelectronics, biological sensors and artificial neural systems (priorities C, D)

National Institutes of Health (NIH)

a. Total FY 2001 request is $36 million, $4 million above FY 2000. Additional $20-30 million will be spent in other targeted programs.
b. Major interests in nanotechnology: Biomaterials (e.g., material-tissue interfaces, biocompatible materials); devices (e.g., biosensors, research tools); therapeutics (e.g., drug and genetic material delivery); infrastructure and training.
c. Estimated funding: approximately $21 million in FY 1999, and $32 million in FY 2000.
d. Modes of R&D support: Academic research; small business research; in-house studies
e. Major themes and new programs in FY 2001 include: – Biomaterials (priority research areas A, B, D listed on page 30)
   - Clinical diagnostic sensors (priorities B, D)
   - Genomics sensors (priorities A, B, D)
   - Nanoparticles and nanospheres for drug and gene delivery (priorities B, D)
   - Multidisciplinary training (priority E)
   - Study social, ethical and legal aspects (priority E)

National Science Foundation (NSF)

a. Total FY 2001 request is $217 million, $120 million above FY 2000.
b. Major interests in nanotechnology: Fundamental research on novel phenomena, synthesis, processing, and assembly at nanoscale; instrumentation, modeling; materials by design; biostructures and bio-inspired systems; nanosystem architecture; infrastructure and education;
c. Estimated funding: $85 million in FY 1999 ($40 million, materials; $14 million, chemistry; $3 million, biology; $25 million, engineering; $1 million, physics; $2 million, information systems); $97 million in FY 2000.
d. Modes of R&D support FY 2001 increment: Individual academic research: $65 million; Grand Challenges $9 million; group and center awards for ERC/MRSEC/STC/National Nanofabrication Users Network including infrastructure: $34 million; Education, training and studies on societal impact: $12 million.
e. Major themes and new programs in FY 2001 include :
   - Nano-biotechnology: biosystems, bio-mimetics and composites (priority A listed on page 30)
   - Nanoscale processes in environment: small length scale/ long time scale processes; functional interfaces between biological/inorganic, inorganic, and biological structures (priority A)
   - New paradigms of operation, synthesis and fabrication: nanostructures “by design”; quantum realm; exploratory computational principles: quantum, DNA, etc. (priorities A, B)

- Integration of systems and architectures at the nanoscale: integration at nanoscale and with other scales; multiscale and multiphenomenal modeling and simulations (priorities A, B, C)
- Multiscale/multi-phenomena at nanoscale (priorities A, B and C)
- Education and training of the new generation of professionals for nanotechnology (priority E)
- Study the impact of nanotechnology on the society at large, including economic, social, ethical and legal considerations (priority E)

Collaborative Activities in the FY 2001 National Nanotechnology Initiative. The NSET will coordinate joint activities that create synergies between the individual agencies in a variety of topics and modalities of collaboration. The coordination will: identify of the most promising research directions, funding of complementary/synergistic fields of research that are critical for the advancement of the nanoscience and engineering field, develop a balanced infrastructure (portfolio of programs, development of new specific tools, instrumentation, simulation infrastructure, standards for nanoscale), correlate funding activities for centers and networks of excellence, cost share high cost R&D activities, develop a broad workforce trained in the many aspects necessary to nanotechnology, study of the diverse, complex implications on society such as effect of nanomaterial manufacturing on environment and effect of nanodevices on health, and avoid of unnecessary duplication of efforts. The coordination also will address NNI management issues.

The coordination has started with the preparation of the IWGN Research Directions in 1999, participation of NSET Subcommittee members at planning activities in each agency in spring 2000, establishment of agency coordinating groups in spring 2000, surveys of the NNI activities of each agency with identification of collaboration opportunities and duplication avoidance, initiation of joint exploratory workshops (such as those on molecular electronics, quantum computing, and nanobiotechnology), and agreements on specific interagency funding programs (such as NASA-National Cancer Institute). Improved internal coordination in large agencies, concurrently with interagency collaboration, has also been noteworthy in the planning process. The coordination addresses issues related to research, infrastructure, societal implications and education and training. The main collaborative activities planned for FY 2001 are:

- *Coordinated research and education activities in all five priority areas listed on page 30. The agency participation in different priorities is shown under each agency on pages 31 to 34.*
- *Focused joint programs* on Grand Challenges and related topics: bioengineering (NIH, NSF, DOD and DOE); unmanned missions (NASA and DOD); lab-on-a chip (NIH, DOE, DOD, NIST, and NSF); quantum computing (DOD, DOE, NASA, NIST and NSF); and environmental monitoring (DOE and NASA).
- *University-based centers* on modeling and simulation at nanoscale, integration of components and devices at nanoscale, nanoscale systems and architectures, nanofabrication, nanotechnology and bio-robotics, and nano-biomedicine (Participants: NSF with STC, MRSEC, ERC, NNUN and other centers, DOD with MUIR, NIH and NASA, state and private organizations)
- *Government laboratory-based user facilities and research networks.* (Participants: All agencies, state and private organizations)
- *An education and training network on nanoscience and engineering* (Participants: all agencies)
- *National facility at NIST for calibration and standards at the nanoscale* (Participants: all agencies)

- *NNI information center for nanotechnology* (Participants: all agencies)
- *Societal implications of nanotechnology* (Participants: NSF, NIH, DOC and other agencies)

Examples of major collaborative NNI activities crossing the participating agencies are shown in Table III.

Table III. Examples of proposed NNI interagency collaborative activities
(subject to funding approval)

Agency	**DOC**	**DOD**	**DOE**	**NASA**	**NIH**	**NSF**
Fundamental research		x	x	x	x	x
Nanostructured materials	x	x	x	x	x	x
Molecular electronics		x		x		x
Spin electronics		x		x		x
Lab-on-a-chip (nanocomponents)	x	x	x	x	x	x
Biosensors, bioinformatics				x	x (1)	
Bioengineering		x	x		x	x
Quantum computing	x	x	x	x		x
Measurements and standards for tools	x	x	x		x	x
Nanoscale theory, modeling, simulation		x	x	x		x
Environmental monitoring			x	x		x
Nanorobotics			x	x		x
Unmanned missions		x		x		
Nanofabrication user facilities	x		x	x		x

(1) NASA and National Cancer Institute (NCI) join effort to develop nano-explorers for the human body (MOU signed on 4/13/00)

The NSET will also reach out to the nanoscience and nanoengineering efforts of other nations in order to take best advantage of knowledge developed by their S&T investments and collaboration opportunities. For example, the NSET will continue its worldwide survey study, the DOD international field offices will start to assess the nanoscience investment strategies and commercial interests in their geographies of responsibility.

Research topics of interest for joint funding include:

- Nanoelectronics and information technology
- Multi-scale, hierarchical modeling and simulation of nanostructures and nanoprocesses

- Development of experimental methods and devices to measure various properties and phenomena at nanoscale; combine measurement, manipulation, and manufacturing tools
- Connection to biology (biostructures and bio-inspired systems)
- Synthesis, assembly, and processing of nanostructured materials "by design"
- System architecture and devices
- Focus on fundamentals that are broadly enabling of many technology areas and that help industry to develop new competitive, profitable products that it would not develop on its own

Partnerships will be encouraged:
- Among disciplines (small group research)
- Among institutions and types of institutions (e.g., universities, industry, government labs)
- Among U.S. Federal government and state funding agencies (support for complementary activities)
- Among expensive equipment users (joint funding and use of facilities in centers)
- Among countries (international collaborations to promote access to centers of excellence abroad, visits by young researchers abroad, and bilateral and multilateral agreements)

Interagency activities for the joint implementation plan will be completed after the funding will be approved. A national nanotechnology coordinating office is being planned. An external board of experts that will evaluate the NNI goals, including the interagency interactions, will be established by the beginning of FY 2001.

Infrastructure Needs for Nanotechnology. A major objective is to create a balanced, predictable, strong, and flexible U.S. infrastructure in nanoscale science, engineering, and technology. This kind of infrastructure is required for the nanotechnology initiative to stimulate further rapid growth of the field. Ideas, concepts, and techniques are developing at an exceedingly rapid pace, such that the field needs coordination and focus with a national perspective. Demands are being made on universities and government to continue to evolve this science and to bring forth the changes in technology that are expected from the field. Even greater demands are on industry to exploit new ideas, protect intellectual property, and develop appropriate products. This field has major transdisciplinary aspects that will be difficult to coordinate without a strategic R&D plan. It is imperative to address these kinds of issues; the future economic strength, quality of life, and national security of the United States may be at stake.

Tools must be provided to investigators in nanotechnology for them to carry out competitive, state-of-the-art research. Tools will include but not be limited to ion, neutron and photon sources, instruments for manipulation, new forms of lithography, computational capabilities, and other systems to characterize the nanoscale systems. Centers involving multiple grantees or laboratories where these tools would be available should be established at a level of several million dollars annually. These centers should also have diverse research teams that will be effective in different scientific disciplines. Means should be investigated to achieve remote use of these facilities. Funding mechanisms should be emphasized that encourage collaboration between centers, university, laboratories, and industry, as well as single investigators who are tied into these networks. A major potential barrier to cooperative efforts is the issue of intellectual property rights, which must be addressed in a national framework.

Support to single investigators for their competence and imaginative programs should provide a corresponding level of personnel and equipment support. University grants should encourage work among research groups to make maximum use of concepts and ideas being developed in other disciplines. The infrastructure must support building of links between researchers, developers, and users of nanotechnology innovations and development of critical enabling technologies that have significant value added in many industries. The focus should be on development of new profitable products that maintain and improve global competitiveness, both short-term (3-5 years) and long-term.

It will be necessary to fund training of students and support of postdocs under fellowships that will attract some of the best students available. This is extremely important, considering the rapid changes in the knowledge base. Students should receive multidisciplinary training in various nanotechnology fields. Both organizational attention and funding should also be devoted to ensuring the open exchange of information in multidisciplinary meetings and to rapid publication of results, through, for example, workshops and widely disseminated summaries of research.

Because of the rapidly evolving nature of nanotechnology and its importance to society, program management must be flexible, with the capability of making changes as necessary. Working groups should be supported to make recommendations to modify the program as it evolves.

IMPLEMENTATION PLAN

8. Implementation of the Proposed Funding Themes and Modes of Support

Funding of the recommended R&D priorities outlined in this document will be conducted by the participating agencies as a function of their mission and contingent on available resources. A coherent approach will be developed for funding the critical areas of nanoscience and engineering, establishing a balanced and flexible infrastructure, educating and training the necessary workforce, and promoting partnerships to ensure that these collective research activities provide a sound and balanced national research portfolio. By facilitating coordination and collaboration among agencies, the NNI will maximize the Federal government's investment in nanotechnology and avoid unnecessary duplication of efforts. The vision, strategy, agency participation, and agency partnerships for the five priorities are described in detail later in this report.

NNI interagency management objectives

NNI will enable agencies to work together collaboratively to meet the primary objective of the initiative: to achieve the maximum National benefit of long term fundamental nanoscale science, engineering and technology research while meeting the mission-oriented technology goals of participating Government agencies. Two overriding management principles will be:

Open competition and/or peer review will ensure that:

- The best ideas for research in nanoscale science, engineering and technology are identified and pursued
- The best individuals and teams are selected to carry out the research
- The best providers of physical and computational infrastructure resources are selected
- Academic, national laboratory, and private sectors - including institutions from all geographic areas, historically minority institutions, and small colleges and universities - have equal opportunities to compete for access to available research and infrastructural resources

Interagency coordination will ensure that:

- Participating agencies work together to address issues that transcend mission objectives
- Resources are leveraged to maximize benefit to NNI, related ongoing research, and agency missions
- The nanotechnology infrastructure is optimized to meet NNI and agency objectives

NNI management plan

The NNI will be managed within the framework of the National Science and Technology Council's (NSTC) Committee on Technology (CT). The Committee, composed of senior-level representatives from the Federal government's research and development departments and agencies, provides policy leadership and budget guidance for this and other multiagency technology programs.

The CT's Subcommittee on Nanoscale Science, Engineering, and Technology (NSET) will coordinate the Federal government's multiagency nanoscale R&D programs, including the NNI. The NSET Subcommittee will coordinate planning, budgeting, implementing, and reviewing the NNI to ensure a broad and balanced initiative. The Subcommittee is composed of representatives from agencies with plans to participate in the NNI and White House officials. The NSET Subcommittee is co-chaired by the White House National Economic Council and a representative from an agency participating in the NNI as designated by the CT. Subcommittee representatives from agencies have operational authority over nanotechnology research and/or nanotechnology infrastructure within their own agency. The NSET Subcommittee succeeds the Interagency Working Group on Nanoscience, Engineering, and Technology (IWGN) as the primary interagency coordination mechanism. Currently, the NSET members are from DOC, DOD, DOE, DOT, EPA, NASA, NIH, NSF, and White House offices (NEC, OMB, and OSTP).

Under the NNI, each agency will invest in those R&D projects that support its own mission as well as NNI goals. While each agency will consult with the NSET Subcommittee, the agency retains control over how it will allocate resources against its proposed NNI plan based on the availability of funding. Each agency will use its own methods for inviting and evaluating proposals. Each agency will evaluate its own NNI research activities according to its own GPRA policies and procedures

National Nanotechnology Coordination Office (NNCO)

A National Nanotechnology Coordination Office (NNCO) will be established to serve as the secretariat to the NSET Subcommittee, providing day-to-day technical and administrative support. The NNCO will support the NSET Subcommittee in the preparation of multiagency planning, budget, and assessment documents. The NNCO will be the point of contact on Federal nanotechnology activities for government organizations, academia, industry, professional societies, foreign organizations, and others to exchange technical and programmatic information. In addition, the NNCO will develop and make available printed and other material as directed by the NSET Subcommittee, as well as maintain the NNI Web Site (http://www.nano.gov).

The NNCO Director will be an NSTC agency representative appointed by the Associate Director for Technology at the White House Office of Science and Technology Policy, in consultation with the Chair of the NSET Subcommittee and Executive Committee of the Committee on Technology. The NNCO Director reports to the Associate Director, but works in close collaboration with the Subcommittee Chair to establish goals and priorities for NNCO support**.**

The NNCO Director will initially be a part-time position. The part-time NNCO Director will be drawn from NNCO sponsoring organizations, on a voluntary basis. The OSTP Associate Director and the part-time NNCO Director's agency will negotiate the expected time commitments and the length of appointment. As the duties and workload of the NNCO expand, the NSET Subcommittee may recommend to the OSTP Associate Director the appointment of a full-time NNCO Director. The full time NNCO Director must be a Federal employee, but recruitment is not limited to NNCO sponsoring organizations. The term of appointment will be established by the OSTP Associate Director, and is not to exceed two years. The appointment of the first part-time NNCO Director will be made the summer of 2000.

Agency detailees and full-time and part-time contractors will staff the NNCO. The NNCO will have a small initial staff (2.5 to 3 FTEs), which will increase only as workload warrants. The NNCO Director will work with the NSET Subcommittee and OSTP in meeting the staffing needs of the Office.

In FY 2001, the NSET Subcommittee will prepare the NNCO budget. The NNCO budget includes the cost of contracting with an outside organization to review NNI progress towards meeting its goals. Beginning in FY 2002 and annually thereafter, the NNCO must submit an annual budget to the NSET Subcommittee for approval. If the NNCO's proposed budget is 15 percent or greater than the previous year, approval by the Executive Committee of the Committee on Technology is required.

Based on an approved budget, the NNCO's annual funding will be derived from cash and in-kind contributions of agencies participating in the NNI based on a percentage of each agency's total (enacted) investment in nanoscale R&D. The percentage may vary slightly from year to year. Agencies can contribute in excess of the amount they have agreed to provide. However, agencies cannot count these extra contributions in one year towards its financial obligations for the following year.

OSTP will work with the NSET Subcommittee and its constituent agencies to develop a Memorandum of Understanding (MOU) which describes the roles and responsibilities, operating procedures, and funding of the NNCO consistent with this memorandum. The NNCO will begin operation once the departments and agencies participating in the NNI have signed the MOU.

<u>Outside Review</u>

In its letter to the President, the PCAST recommended that a non-government advisory committee review the NNI annually to assess progress towards its goals. A report would be provided to the Committee on Technology. The Committee would work with the NSET Subcommittee to address issues raised by the outside advisory committee and to implement changes to the NNI strategy. Initial discussions on such an advisory committee have been held between the members of the Committee on Technology and the National Research Council.

Coordination

NNI coordination will be achieved though the NSET Subcommittee, direct interactions among program officers within participating agencies, periodic management meetings and program reviews, and joint science and engineering workshops. The NSET Subcommittee will coordinate joint activities among agencies that create synergies or complement the individual agencies' activities to further NNI goals. Communication and collaborative activities are also facilitated by the NNI website as well as by the agencies' sites dedicated to NNI.

Examples of NNI coordination include identification of the most promising research directions, encouraging funding of complementary fields of research across agencies that are critical for the advancement of the nanoscience and engineering field, education and training of the necessary workforce, and establishing a process by which centers and networks of excellence are selected.

The NNI coordination process began in 1999 with the preparation of the IWGN Nanotechnology Research Directions. In the spring of 2000, NSET Subcommittee (formerly IWGN) members participated in planning activities at each agency. In addition, a survey is being conducted in all agencies participating in the NNI to identify opportunities for collaboration and areas where duplication can be avoided. Discussions are being held regarding joint exploratory workshops (such as those on molecular electronics, quantum computing, and nanobiotechnology), and agreements on specific interagency funding programs. Improved internal coordination in large agencies, concurrently with interagency collaboration, has also been noteworthy in the planning process.

Examples of major collaborative NNI activities planned by the participating agencies are:

Agency	**DOC**	**DOD**	**DOE**	**NASA**	**NIH**	**NSF**
Fundamental research		x	x	x	x	x
Nanostructured materials	x	x	x	x	x	x
Molecular electronics		x		x		x
Spin electronics		x		x		x
Lab-on-a-chip (nanocomponents)	x	x	x	x	x	x
Biosensors, bioinformatics				x	x	x
Bioengineering		x	x		x	x
Quantum computing	x	x	x	x		x
Measurements and standards for tools	x	x	x		x	x
Nanoscale theory, modeling, simulation		x	x	x		x
Environmental monitoring			x	x		x
Nanorobotics			x	x		x
Unmanned missions		x		x		
Nanofabrication user facilities	x		x	x	x	x

The NSET Subcommittee will reach out to the nanoscience and nanoengineering efforts of other nations. These emerging fields create a unique opportunity for the U.S. to partner with other counties in ways that are mutually beneficial. Potential activities include information sharing, cooperative research, and study by young U.S. scholars at foreign centers of excellence. In addition, the NSET Subcommittee will continue its worldwide survey study, DOD's international field offices will assess the nanoscience investment strategies and commercial interests in their geographies of responsibility.

Time line summary

Table IV lists NNI key deliverables in the next five years. Out-year deliverables depend on regular increases in funding for this initiative.

Table IV. NNI key deliverables in the next five years (Fiscal years 2001 - 2005)

Deliverable	***First Achieved***
Begin augmented research and development in fundamental research, grand challenges, infrastructure, education and nanotechnology societal impacts in response to open competitive solicitations and regular program reviews	FY 2001
Begin work on teams and centers for pursuing mission agency objectives	FY 2001
Establish ten new centers and networks with full range of nanoscale measurement and fabrication facilities	FY 2002
Develop five new standard reference materials for semiconductors, lab-on-a-chip-technologies, nanomagnetics, and calibration and quality assurance analysis	FY 2003
Develop standardization systems for nanocharacterization, nanomanipulation and nanodevices	FY 2004
Develop quantitative measurement methods for nanodevices, nanomanipulation, nanocharacterization and nanomagnetics; Develop several 3-D measurement methods for the analysis of physical and chemical at or near atomic spatial resolution.	FY 2004
Ensure that 50 % of research institutions faculty and students have access to full range of nanoscale research facilities	FY 2005
Enable education access to nanoscience and engineering for at least 25% of students in research institutions	FY 2005
Catalyze creation of several new commercial markets that depend on three-dimensional nanostructures	FY 2005
Develop three-dimensional modeling of nanostructures with increased accuracy that would allow simple system and architecture design	FY 2005

9. Fundamental Research

(total investment proposed for FY 2001 is $177 million, $90 million above FY 2000)

Vision and Strategy

The National Nanotechnology Initiative identifies five "high priority" research areas for additional funding beginning in FY2001. The first and largest of these is "long-term science and engineering research leading to new fundamental understanding and discoveries of phenomena, processes, and tools for nanotechnology". The investment will provide sustained support to individual investigators and small-groups, with a typical award of $200K to $500K. Sustained and larger funding for fundamental research in the early years of the Initiative is critical for its success.

Vision

The Initiative will develop the capacity to create affordable products with dramatically improved performance through gaining a **basic understanding of ways to control and manipulate matter at the ultimate frontier – the nanometer** – and through the incorporation of nanostructures and nanoprocesses into technological innovations. In addition to producing new technologies, the study of nanoscale systems also promises to lead to fundamentally new advances in our understanding of biological, environmental, and planetary systems.

Nanoscience is still in its infancy, and only rudimentary nanostructures can be created with some control. The science of atoms and simple molecules, on one end, and the science of matter from microstructures to larger scales, on the other end, are generally established. The remaining size-related challenge is at the nanoscale, roughly between 1 and 100 molecular diameters, where the fundamental properties of materials are determined and can be engineered. A revolution has been

occurring in science and technology, based on the recently developed ability to measure, organize, and manipulate matter on a scale of 1 to 100 nanometers (10^{-9} to 10^{-7} m) and on the importance of controlling matter at nanoscale on almost all human-made products. Recently discovered organized structures of matter (such as carbon nanotubes, molecular motors, DNA-based assemblies, quantum dots and molecular switches) and new phenomena (such as magnetoresistance and size confinement) are scientific breakthroughs that merely indicate future potential developments. Nanotechnology creates and utilizes functional materials, devices, and systems by controlling matter on this scale.

Nanotechnology promises to be a dominant force in our society in the coming decades. The few commercial inroads in the hard disk, coating, photographic, and pharmaceutical industries have already shown how new scientific breakthroughs at this scale can change production paradigms and revolutionize multibillion dollar businesses. Formidable challenges remain, however, in fundamental understanding of systems on this scale before the potential of nanotechnology can be realized. An acceleration of the pace of fundamental research in nanoscale science and engineering will allow for development of the necessary knowledge and human and technological base. Currently, Federal agencies are not able to support many research requests in nanosystems, nano-bioengineering, quantum control, nanosimulations, and nanoscale processes in the environment. Also, there is a need for interdisciplinary consortia that will integrate various disciplines and university/industry/national laboratories' efforts in nanoscience and engineering.

There are several reasons why the nanoscale is so interesting and important:

- Electronic and atomic interactions inside matter are influenced by variations at the nanometer scale. Patterning matter at a nanometer length scale will make it possible to control the fundamental properties of materials (such as magnetization, charge capacity, catalytic activity) without having to change their chemical composition. For instance, nanoparticles of different sizes emit light at different frequencies so they can be used for different color, and nanoparticle are of the size of single magnetic domains so vastly improved magnetic devices can be made.
- Because systematic organization of matter at nanoscale is a key feature of biological systems, nanoscience and technology will allow us to place artificial components and assemblies inside cells and to make new structurally organized materials by mimicking the self-assembly methods of nature. These materials and components will be more biocompatible.
- Nanoscale components have very high surface areas, making them ideal for use as catalysts and other reacting systems, adsorbents, drug delivery, energy storage, and even cosmetics.
- Many nanostructured materials can be harder, yet less brittle than comparable bulk materials with the same composition because of certain interface and confinement effects. Nanoparticles or nanograins are too small to have surface defects and are harder because of the surface energy so they can be used to make very strong composite materials.
- The speed of interacting nanostructures is much faster than that of microstructures because the dimensions involved are orders of magnitude smaller. Much faster and energy efficient systems are envisioned.

As Feynman sagely pointed out in 1959, nanoscience is one of the unexplored frontiers of science. It offers one of the most exciting opportunities for innovation in technology. It will be a center of fierce international competition when it lives up to its promise as a generator of technology.

Special Research Opportunities

The nanoscale is not just another step towards miniaturization, but a qualitatively new scale. The new behavior is dominated by quantum mechanics, material confinement in small structures, large interfaces, and other specific properties and phenomena because of the size. Many present theories of matter at microscale have critical length of nanometer dimensions; these theories will be inadequate to describe the new phenomena at nanoscale.

Long-term, basic research opportunities arise in

- Developing scaling laws, and threshold length and time scales for the properties and phenomena manifested in nanostructures.
- Linking biology, chemistry, and physics to accelerate progress in understanding the fundamental principles behind living systems and the environment.
- Discovering and eventually tailoring the novel chemical, physical, and biological properties and phenomena associated with individual and ensembled nanostructures being anticipated.
- Creating new instruments with the sensitivity and spatial localization to measure, manipulate, and able to *in-situ* monitor processing of nanostructures; utilizing the new ability to measure and manipulate supramolecules to complement and extend prior measurements derived from ensemble averages.
- Addressing the synthesis and processing of engineered, nanometer-scale building blocks for materials and system components, including the potential for self-organization and self-assembly.
- Exploiting the potential for both modeling/simulation and experiment to understand, create and test nanostructures quantitatively.
- Developing new device concepts and system architecture appropriate to the unique features and demands of nanoscale engineering.

Priorities and Modes of Support

Long-term nanoscale research should be focused on understanding basic processes for the new ranges of length and time scales, on development of new measurement and manipulation tools, and on development of the processes necessary to fabricate quality nanostructures in areas of maximum potential impact on technology, health, national security, and the environment. Areas of focus include the following:

- *Biosystems at the nanoscale*: Study of biologically based or inspired nanoscale systems that exhibit novel properties and potential applications will include study of the relationship, on this scale, among chemical composition, physical shape, and function. Potential applications include improved drug and gene delivery, biocompatible nanostructured materials for implantation, artificial photosynthesis for clean energy, and nanoscale sensory systems, such as miniature sensors for early detection of ovarian cancer.
- *Nanoscale structures and quantum control*: Computing, communications, and information storage technologies will approach physical limits of miniaturization as feature sizes in electronic devices reach the nanoscale level. Novel phenomena at the quantum limit that must be explored, understood, and exploited in order to overcome barriers will appear on this scale. New tools will be needed for molecular scale synthesis and processing, fabrication, manipulation, and control. Potential applications include the development of new processes

across the entire range of communications and information technology, including ‘quantum computing’.

- *Device and system architecture*: Research is needed to develop new concepts and investigative tools for nanostructured device concepts and system architectures, to understand the interfaces and dynamics of interacting nanostructures, to control complexity, and to simulate nanostructure assemblies like sensors and nano-motors. Potential applications include integrated devices to monitor health, interconnected nanoscale mechanical and electronic circuits, and multifunctional ‘smart’ devices that can change physical properties in response to external stimuli for safety, space, and national security applications.
- *Nanoscale processes in the environment*: The role and impact of nanoscale phenomena in the environment is only beginning to be realized. Research is needed to develop and adapt new experimental, theoretical, and computational approaches for characterizing nanostructures in the environment and to develop an integrated understanding of the role of nanoscale phenomena in ecosystems. Potential applications include pollution control and understanding the origins of biodiversity. Because natural and artificial nanoparticles can be trapped in lungs, the nanoparticle generation and transport need to be investigated.
- *Multiscale/multiphenomena modeling and simulation*: The emergence of genuinely new phenomena at the nanoscale creates a great need for theory, modeling, and large-scale computer simulation in order to understand new nanoscale phenomena and regimes. The links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are not understood well, although for the simplest semiconductor systems, carbon nanotubes, and similar “elementary” systems, considerable progress has been made. However, for more complex materials and hybrid structures, even the basic outline of a theory describing these connections remains to be written. In nanoscale systems, thermal energy fluctuations and quantum fluctuations are comparable to the activation energy scale of materials and devices, so that statistical and thermodynamic methods must include these effects more fully. Thus, the performance of nanoscale devices depends on stochastic simulation methods, as well as computational models incorporating quantum and semi-classical methods for evaluation. Consequently, computer simulations, both electronic-structure-based and atomistic, will play a major role in understanding materials at the nanometer scale and in the development “by design” of new nanoscale materials and devices. The greatest challenge and opportunity will be in those transitional regions where nanoscale phenomena are just beginning to emerge from macroscopic and microscale regimes that are describable by bulk property theories combined with the effects of interfaces and lattice defects.

Nanoscale science and engineering is inherently interdisciplinary. A focus on interdisciplinary teams of researchers and on exploratory research projects is recommended. Active collaboration between academic and industrial scientists and engineers, and integration of research and education will be encouraged. Interagency partnerships will play a synergistic role in these activities.

Impact on Infrastructure

The research activities will use and help develop a laboratory and human resource infrastructure for nanotechnology. A skilled workforce familiar with the tools and concepts of nanoscience will be established for moving scientific breakthroughs from the laboratory to practical application.

Agency Participation and Partnerships

NSF will contribute the largest investment to this generic fundamental research topic. While DOD, DOE, NASA, and NIH will primarily address the fundamental research issues inherent in their Grand Challenges, they will also contribute to generic fundamental research as a way to retain flexibility. Both academic institutions and government research laboratories will conduct fundamental research. Coordinated research and education activities in all five priority areas listed on page 30 are planned.

NSF will support research at the frontier of nanoscience and engineering, with a focus on bionanosystems, quantum control in nanostructures, device and system architecture, nanoscale processes in environment, and modeling and simulation at nanoscale. About 67% of awards will be made in open competition in the broad-based NSF programs. A FY 2001 NSF-wide initiative will invest about 33% of the funds on interdisciplinary small-group proposals, centers and networks of excellence in nanoscale science and technology. Participating directorates include the Biological Sciences, Computer and Information Sciences and Engineering, Engineering, Directorate for Geosciences, and Mathematical and Physical Sciences. This level of investment will strengthen critical fields and help to establish the science and engineering infrastructure and workforce needed to exploit the opportunities presented by these new capabilities.

DOE will establish a portfolio of programs balanced in scope and in size, ranging from individual principal investigators to large groups. Proposals will be encouraged from relatively small groups of a few principal investigators at universities and/or national laboratories as well as from larger groups focused on particular problems such as might be appropriate for a university center, a national laboratory, or a user facility. Interactions among scientists with a diverse set of skills in areas such as molecular design, synthesis and assembly, molecular modeling, instrumentation development, theory and modeling, and device engineering will also be encouraged. Involvement of young investigators - graduate students, postdoctoral research associates, and young faculty and staff - with appropriate expertise is critical to the success of the science and to the evolving future of this field. Interactions among several institutions, including both academic and national laboratory partners, is expected to occur naturally for each of the major focus areas. All BES activities will be peer reviewed following broad solicitations for proposals. DOE (through its Office of Industrial Technologies) will support some industry/National Lab/University partnerships for nanotechnology development of use to basic industries.

DOD will provide $10 million ($4 million over FY 2000) for fundamental research. The additional funds for nanoscience and technology ($40 million over FY 2000) are allocated to two separate budget lines: $30M DUSD (S&T) URI, OSD and $10M to Navy Basic Research. This breakout was chosen consonant with the goal of providing approximately 75% of the research funding to University investigators; the OSD URI budget line can fund only university research. Since a goal of the NNI is augmented collaboration amongst university/industry/government, the ONR budget line is available so that DOD laboratories and industry can participate.

DOD participated in the NIH planning for the Bioengineering Consortia (BECON) symposium on Nanoscience and Nanotechnology Shaping Biomedical Research. Since NIH has far greater resources in biology/medicine, the DOD investment in nanobiotechnology must be closely coordinated with NIH. DOD has also been working with NSF on a potential simulation/modeling

effort that would complement the recent BAA announcement NSF 00-36 “Nanoscale Modeling and Simulation”; the historical DOD attention to high performance computing makes this opportunity particularly promising.

NASA looks to NSF and other agencies’ basic science sponsored work for wide-ranging contributions in fundamental research, and expects to allocate only a modest portion (10-20%) of its program to basic research, emphasizing work in direct support of the grand challenge areas the agency selects for focus.

NIH will support nanotechnology research that has exceptional promise to lead to new tools for the diagnosis of disease, novel therapeutic solutions, and enhanced research methods in biology. Very little is known today about how to harness the rudimentary concepts and tools developed by nanotechnologists from other disciplines, for uses in biology and medicine. It is probably true that the most important ways in which nanotechnology will ultimately contribute to biomedicine cannot even be foreseen today. NIH maintains active liaison to other government agencies involved in NNI (i.e. DOE, NSF, NIST, NASA, DOD) through BECON and other trans-NIH working groups, and through specific programs within the Institutes and Centers. Representatives to two of the NNI agencies are participating members of BECON and two BECON members are NIH representatives to NSET Subcommittee.

10. Grand Challenges

(total FY 2001 is $133 million, $62 million above FY 2000)

The following Grand Challenges have been identified as essential for the advancement of the field: nanostructured materials "by design"; nanoelectronics, optoelectronics and magnetics; advanced healthcare, therapeutics and diagnostics; nanoscale processes for environmental improvement; efficient energy conversion and storage; microspacecraft exploration and industrialization; bio-nanosensors for communicable disease and biological threat detection; economical and safe transportation, and national security.

Nanostructured Materials “by Design” — Stronger, Lighter, Harder, Self-Repairing, and Safer

Vision and Strategy

Vision

The initiative will support new generations of innovative materials that exploit the organization of matter at nanoscale and that are high performance yet affordable, able to adapt, and more environmentally benign. The novel materials will be created for given purposes and may be multifunctional, may sense and respond to changes in surroundings, may be ten times stronger than steel, may be ten times lighter than paper, may be paramagnetic or superconducting, optically transparent, and may have a higher melting point. The new materials may combine best properties of two or more known structures.

Special Research Opportunities

Nanostructured materials have smaller structures than most of current materials, and this has an important qualitatively effect under a threshold small size. A typical current structure is composed of groups of many trillions of molecules. Nanotechnology involves groups of a few or even single molecules. This difference fundamentally changes the way nanostructured materials behave and opens entirely new and radically different applications. Major differences between the ways nanostructured materials and conventional materials behave result from nanostructured materials' much larger surface area per unit volume and the confinement effects within each material entity. Since many important chemical and physical interactions are governed by surfaces, a nanostructured material can have substantially different properties than a larger material of the same composition. Compared to conventional materials, nanostructured materials yield extraordinary differences in rates and control of chemical reactions, electrical conductivity (nanostructured materials can be highly conductive, highly insulating, or semiconducting), magnetic properties, thermal conductivity, strength of bulk substance made of nanoparticles (resistance to fracture or deformation, elasticity, ductility, etc.), and fire safety.

To make nanostructures, we must learn to design and manufacture structures that are correct at the atomic and single molecule level. The synthesis and formation of individual nanostructures have many promising opportunities, including dendritic polymers, block copolymers, sol-gel chemistry and controlled crystallization, aerosol nucleation, modified condensation, and nanotube growth. Research into self-assembly, net-shape forming, templating, and other manufacturing approaches will allow for a high level of control over the basic building blocks of all materials. An important challenge is to scale up the laboratory processes and develop commercially viable production methods to manufacture stable nanostructures. The creation of new materials will make extensive use of molecular modeling and simulation. High performance computing now permits simulations based on first physico-chemical principles with few molecules, and these capabilities are expanding rapidly. Another challenge is to develop a single simulation that includes multiple length scales.

The properties of individual nanostructures must be quantitatively measured to establish differences from bulk properties. But the real challenge is to investigate the properties of percolating structures (nanostructure networks) and matrix isolated nanostructures where the impacts of neighboring grain interactions begins to modify nanostructure properties. As we move from the individual nanostructure to networks, composites, and coatings, the admixtures of different nanostructures into an integrated entity will benefit from the unique contributions of the different components.

Compacting nanostructures offers another opportunity. The properties of nanostructure interfaces can be unique in themselves. For instance, nanopowder compacts offer high strength simultaneously with ductility. Techniques to make these compacts in bulk and coating forms are necessary; control of the interface composition/structure is crucial. This opportunity could yield coatings for reduced life-cycle-cost, net-shape forming structures for reduced manufacturing costs, and many other improvements.

High surface area materials provide another perspective on nanostructures — controlled porosity where the nanostructure is open space enveloped in a thin material structure. Aerogels and zeolites offer two examples. These materials offer important opportunities in chemical synthesis (hetero-

catalytic reactions), clean-up (adsorbents), and separation (controlled porosity membranes) with expected applications in the chemical industry, environmental clean up, and biotechnology.

Relevance
Performance advances of materials have impact on broad commercial, standard of living and national security aspects. Nanostructuring leads to the next generation of high performance materials. Areas of impact include:

- Materials that are much *harder, stronger, more reliable, and safer* so that they last many times longer than our current technology allows will make bridges, roads, road signs, and traffic control systems — helping our tax dollars go farther. The means of transportation by ground, water and air spacecraft need lightweight, long-lived, yet strong materials: strength for function and safety, low weight for fuel economy and agility, and low failure rates (wear, corrosion, fracture, and fatigue) for life-cycle cost and waste reduction. Present military/space platforms have material limitations on their duration and performance that are clearly deleterious to mission success. The importance of better gas mileage will increase with the diminution in oil supply, expected in 10-20 years. Safety requirements in transportation will lead to introduce smart furniture fabrics with nanodesign and high strength nanostructured plastics that do not burn. New polymer and nanocomposite materials will not only be many times stronger, but they will prevent fires from spreading and dramatically reduce the production of toxic fumes.
- With the incorporation of sense/response functions directly into materials, these *smart materials* will have condition-based maintenance (reducing the enormous cost of multibillion $/year associated with materials replacement) and will provide new materials capabilities. One military application would be stealthy materials that can recognize probing radar or sonar beams and initiate an action that gives no return signal. Automobile and aircraft materials could also be made to sense incipient failure and warn the user well in advance, rather than stranding him on the highway or plunging her from the air. Paints that change color with temperature — white when hot (solar reflective) and black when cold (solar absorptive) — could provide home heating or cooling adjustments. *Smart windows* in the home and workplace will create huge energy savings.
- Nanotechnology will potentially lead to long lasting, self-cleaning surface finishes; reducing friction, wear, and corrosion; and providing multispectral camouflage (visible, infrared, millimeter wave, radar, and sonar).
- In medical applications**,** nanomaterials will make self-regulating pharmaceutical dispensers compatible with biosystems so that they will not be rejected by the human body and will last many times longer in the corrosive and mechanically harsh environment of the human body.

Materials manufacture and disposal contribute substantially to environmental problems. Nanotechnology offers new biodegradable structures that can be designed for chosen functions**.** Self-assembly and/or final shape forming *of* manufactured nanostructures will have less waste by-product than the cutting operations presently used in manufacturing. Longer-lived materials — reduced wear corrosion, fatigue, and fracture though nanostructure control — will reduce the amount of material to dispose.

Priorities and Modes of Support

Nanostructured materials offer a wide range of investment opportunities, with the following expecting to lead to good future return on investment:

- Develop synthesis, processing, and fabrication methods for nanostructures like nanoparticle powders and nanotubes from inorganic and organic materials, and scale up these methods for industrial uses
- Develop models and simulations that incorporate all size scales from nano to macro and that predict materials performance
- Extend the range and sensitivity of analytical tools that measure the composition, structure, and properties of individual nanostructures and their various aggregated forms (networks, composites, coatings, compacts)
- Measure the properties of individual nanostructures, percolating structures (nanostructure networks), and matrix isolated nanostructures. The latter two provide a high degree of design freedom for potential applications such as dielectrics for electromagnetic absorbers, sensors, detectors, and converters
- Develop nanostructured fillers embedded in a matrix; for instance, nanotubes for strength, nanoclay for fire, nanocarbons for wear resistance, tailored "pigment" incorporation for multispectral low observable structures and materials, including a focus on interfacial properties between filler and matrix
- Develop nanostructured nanoparticles consolidated into composites and nanoporous materials where control of porosity holds promise for chemical selectivity in adsorption, permeation, and chromatographic applications
- Understand the physics and control of nanoscale failure initiation mechanisms

Single investigator projects will dominate the investment portfolio, but selected centers will be necessary to fund expensive equipment.

Infrastructure

Centers and networks will be crucial for nanostructure characterization. The National Laboratory synchrotron and neutron facilities will be important for the range of wavelengths (sub-nanometer to thousands of nanometers) since they provide diffraction/scattering characterization for various length scales. Academic centers with high-resolution electron microscopes (HREM) and other high cost analytical tools will be necessary.

<u>Agency Participation and Partnerships</u>

All agencies, with larger contributions from DOD, DOE, DOC and NASA, will move toward materials issues that address their mission needs and will partner with NSF to establish the generic science base.

Examples: DOE's design and synthesis of materials at the atomic level for desired properties and functions. In the future, design and synthesis of new materials at the atomic level will be accomplished using only the electronic structure of the elements. Because of the small dimensions, it will be possible in many cases to calculate the desired properties of materials knowing only the atoms that make the material. In cases where simulation is not possible, powerful experimental combinatorial approaches can be used to vary conditions and compositions and search for materials with new or improved properties. Large numbers of differing

samples can be made and tested very quickly. These experimental approaches will be especially important for structures that are not at equilibrium, that might include small amounts of minor constituents, and that might be prepared using extreme conditions such as high pressure or high magnetic fields. A very important part of the research for this goal is the synthesis of molecular building blocks that will lead to functional materials and the design of molecular machines from molecular building blocks.

NASA's focus in this area is on high strength-to-mass, "smart" structural materials in the context of: Safer, more reliable, multifunctional and eventually self-repairing aerospace vehicle structures; smart and agile materials with programmable optical, thermal and/or mechanical properties; high-precision, low-mass, very-large optical elements with active surface figure control, and self-cleaning surface finishes; ultra-large space structures such as antennas, solar sails and gossamer spacecraft; materials for special environments, e.g. low/high temperature, low/high pressure, low/high gravity, high radiation and chemically reactive. DOD and NASA have overlapping interests in large space optics and antennas, and high-strength-to-mass aerospace structural materials in general.

Nano- Electronics, Optoelectronics and Magnetics

Vision and Strategy

Vision

Nanometer structures will foster a revolution in information technology hardware rivaling the microelectronics revolution begun about 30 years ago that displaced vacuum tube electronics. Minuscule transistors and memory chips will improve computer speed and efficiency by factors of millions, expand mass storage electronics to multi-terabit memory capacity that will increase the memory storage per unit surface a thousand-fold and make data available on a pinhead, and reduce power consumption tens of thousands of times. Communication paradigms will change by increasing bandwidth a hundred times — which will reduce business travel and commuting — and by developing foldable panel displays that are also ten times brighter. Merging biological and non-biological objects into interacting systems will create new generations of sensors, processors, and nanodevices.

Special Research Opportunities

The cost of a single fabrication plant for 70 nm nanometer microelectronics is estimated at over $10B. It is necessary to identify synthesis, processing, and manufacturing approaches for commercially affordable nanostructures, such as printing and stamping approaches to pattern transfer, innovations in surface processing, controlled nucleation, directional growth, and directional etching. Other approaches under consideration are individual atom and molecule manipulation, batch formation of precursor nanostructures (powder, cluster, colloid, nanowires, nanodots, fullerene/nanotubes), directed self-assembly whereby individual nanostructures aggregate, and parallel processing via arrays of microfabricated proximal probes.

An investment must be made to accelerate progress in measurement capabilities — electronic, optic, magnetic, and other properties essential to device design; chemical and structural analysis for fundamental understanding and control; the integration of tools for simultaneous, multiple property measurements on the same structure; and techniques compatible with *in situ* fabrication processes.

Novel device concepts must be established. Nanodevices require understanding fundamental phenomena, the synthesis of appropriate materials, the use of those materials to fabricate functioning components, and the integration of these components into working systems. For this reason, success will require a substantial funding level over a long period of time. Exploratory research is necessary on quantum size effects, tunneling, exchange coupling, and other phenomena where present physical models have critical scale lengths larger than the size of the structure. The desirability of room temperature operation will be a severe constraint, but nanostructures promise materials stable at room temperature that can be manipulated. Examples of innovative device concepts include single electron devices, spin-electronics, resonant tunneling devices, quantum dots, molecular electronics, and vertical cavity lasers.

The new properties of nanostructures and the requirements for quality control for large numbers of small nanodevices in a system will necessitate innovative approaches to information system architectures. Examples include cellular automata, quantum computers, cellular parallel computers, neural networks, photonic crystals, computation using DNA, and mechanical molecular memory.

Our ability to control materials in one dimension to build nanometer scale structures with atomic scale precision in now-commercial giant magnetoresistance devices comes from a decade of basic and applied research on thin film growth, surfaces, and interfaces. The extension from one nanodimension to two or three is not straightforward, but the payoffs can be enormous.

In all of the above opportunities, modeling and simulation will play an essential role. As one gains control of matter at the nanometer scale, the possible combinations and permutations of structures become far too great for only experimental approaches to progress.

Relevance

Nanodevices will extend the U.S. lead into hardware for information technology and other nanodevice use. For example, the goal of microspacecraft guarantees strong attention by the space community. Revolutionary advances in medicine for disease control and in defense for combat knowledge superiority fields are envisioned.

The Semiconductor Industry Association (SIA) roadmap projects nanotechnology to 0.1 micron by approximately 2010, then terminates; it states that new materials, new technologies, affordable scaling, and new approaches <u>must</u> be invented and that these required inventions constitute a Grand Challenge. The year 2010 is only ten years away; now is the time for government investment in the nanoscience base that will enable information nanotechnology.

Priorities and Modes of Support

The research interests should be focused on the following:

- New approaches to nanostructure synthesis and processing that will lead to affordable commercial fabrication
- The physics of innovative device concepts
- New systems and architectures for given functions

- Multiscale/multiphenomena modeling and simulation of complex systems with focus on information technologies
- New optical properties achieved by fabricating photonic band gap superlattices to guide and switch optical signals with nearly 100% transmission, in very compact architectures

A strong, single investigator program is essential to introduce the broad range of innovations necessary to this Grand Challenge. But there is also the need for multidisciplinary centers — combining physics, chemistry, electrical engineering, computational science, and other traditional academic departments. The centers should be charged with integrating industrial and academic interests.

Infrastructure

Instrumentation and facility centers — incorporating not only the expensive items such as high voltage, high-resolution electron microscopes, but also suites of proximal probes —will be necessary for full characterization capability. These centers must provide competent, affordable assistance to visiting users. They must also develop new instrumentation that eliminates the many deficiencies in the present capability. The National Nanofabrication Network will need expansion and enhancement.

<u>Agency Participation and Partnerships</u>

All agencies, with particular attention by DOD, DOE, NASA, and DOC/NIST for mission driven projects and NSF for fundamental aspects. Partnerships between university/government/industry will be essential to the rapid transition of nanostructure science into new information technology hardware. The DOD/MARCO and DOD/EPRI Government-Industry Co-sponsorship of University Research (GICUR) research center programs are an example of this needed partnership.

Examples: NIST's nanomagnetic materials R&D: The magnetic data storage industry is an example of the widespread commercialization of nanotechnology. Magnetic storage bits on new computer hard disks currently measure 80 nanometers by 500 nanometers, and read/write head flying distances are only 20 nanometers. The trend in information storage continues toward higher information density and higher access speed, both of which double every two to three years. NIST proposes to work in the areas: magnetic bit stability and kinetics in thin films, imaging methods for nanomagnetics, and physical standards for magnetic measurements. This project will produce standards for films having a magnetic moment 100,000 times smaller than references now available from NIST.

NASA will invest in the following areas: quantum-limited sensors of electromagnetic radiation and fields; low-power, ultra-high-speed signal processing devices and computers; high-density, radiation-tolerant memory technologies; devices for special environments, e.g. low/high temperature, low/high pressure, low/high gravity, high radiation and chemically reactive. DOD and NASA have overlapping interest and will collaborate in radiation tolerant devices and new architectures for ultra-high-speed space-based computing.

Advanced Healthcare, Therapeutics and Diagnostics

Vision and Strategy

Vision
Nanotechnology will contribute to major advances in healthcare through the development of biosensors and new imaging technologies that will allow earlier detection of cancer and other diseases; more effective, less expensive diagnostics and therapeutics using rapid gene sequencing; novel biocompatible materials that will double the retention time of artificial organs; targeted gene and drug delivery systems; enable vision and hearing aids; and use of tiny "smart" medical devices for treatment modes that will minimize collateral damage of human tissues.

a. Earlier Detection and Treatment of Disease

Special Research Opportunities
Nanotechnology will play a central role in the development of new technologies to detect and treat disease much earlier. Current approaches to healthcare for most diseases depend on the appearance of substantial symptoms before medical professionals can recognize that the patient has the disease. By the time those symptoms have appeared, effective treatment may be difficult or impossible. Earlier detection of incipient disease will greatly enhance the success rate of existing treatment strategies and would significantly advance our ability to employ prevention strategies that could arrest or delay the onset of clinical symptoms that may require chronic treatment and/or intervention. Nanoscience and technology will play a central role in the development of novel methods for detecting the biological and structural evidence of incipient disease.

Priorities
- Improved medical imaging technology

Medical imaging today uses X-rays, magnetic resonance, and ultrasound imaging. These technologies have an impressive ability to report, non-invasively, on structures within the body. However, they have not yet reached the speed, low cost, resolution, and sensitivity that their practitioners strive for; and as a result, most diseases and conditions must be relatively advanced before they can be detected. Advances that nanotechnology will bring to other fields such as electronics and computing will directly benefit medical imaging. Nanotechnology will also result in improved contrast agents for use in conjunction with imaging systems. Delivery of conventional contrast agent molecules to sites in the body that are currently inaccessible to those molecules will be achieved through the use of small particles designed to have the physical and chemical properties consistent with delivery to their target organ. New chemical and particulate formulations will also be created to enhance the images created by such imaging modalities as MRI and ultrasound.

As a result of these improvements, diseases will be detectable earlier than they are today: Tumors consisting of just a few cells, or subtle perturbations to blood flow that signal a warning of impending heart disease, will be detectable, making earlier treatment possible.

- Sensors

Implantable sensors or 'smart' patches will be developed that can monitor patients who are at risk for specific conditions. Such sensors might monitor, for example, blood chemistry, local electric

signals, or pressures. The sensors would communicate with devices outside the body to report results, such as early signals that a tumor, heart damage, or infection is developing. Or these sensors could be incorporated into "closed loop" systems that would dispense a drug or other agent that would counteract the detected anomaly. For chronic conditions like diabetes, this would constitute a great leap forward. Nanotechnology will contribute critical technologies needed to make possible the development of these sensors and dispensers.

- Susceptibility Testing

Sensor systems that can rapidly process patient samples and detect an array of medically relevant signals at high sensitivity and selectivity will also be developed for the clinical laboratory or doctor's office. Some of these tests will be based on nucleic acids like DNA or RNA and will be used, for example, to rapidly determine a patient's susceptibility to certain diseases, infections, toxins, etc. Knowledge of this information will help the patient make lifestyle and employment decisions and watch for those diseases likely to affect them. More effective, more personalized treatments will come with the ability to use DNA profiles to classify patients according to their responsiveness to certain pharmaceutical drugs or to their potential for having adverse reactions to particular pharmaceuticals. Current technology leads toward such tests/devices, but nanotechnology will expand the options leading to greater sensitivity and far better efficiency and economy.

b. Improved Implants

Special Research Opportunities

Artificial organs or organ-assist devices require implantable materials both compatible with the biological environment and resilient to the chemistry of that environment. Better materials and understanding of their interactions with the body may lead to implants that the body will not only accept but will actually become integrated into the body. Nanometer scale surface modifications offer potential for creating novel structures that will allow scientists to control interactions between materials and biological systems.

It is clear that effective manipulation of biological interactions at the nanometer level can dramatically improve the functionality and longevity of implanted materials. For example, titanium implants used today for orthopedics and in dentistry become encapsulated with dense fibrous tissue. This tissue creates an uneven stress distribution at the implant-bone interface, which can result in implant loosening and failure, and even fracture the adjacent bone. By applying "bioactive" thin (nanoparticle) coatings on the surface of the implants, it will be possible to bond the implant more naturally to the adjoining bone and significantly improve the implant lifetime. Future fundamental discoveries in nanoscience, biology, chemistry, and instrumentation will provide the basis for the development of materials that will overcome the challenges implicit in the design and creation of novel biocompatible materials with broad biomedical applications.

c. Nanotechnology for Therapeutic Delivery

Special Research Opportunities

The challenge is to develop and deploy nanoparticles for delivering drugs, gene therapies, and other therapeutics. These technologies will deliver drugs or other molecules that are hard to dissolve and

may even deliver them directly to their site of action. Such nanoparticles will be used to treat cancer and a wide range of other diseases.

Many drugs that work well in the test tube fail in the body because they will only dissolve in fluids that cause undesirable side effects or become trapped in other parts of the body than where they are needed. Evidence has shown that drugs whose chemical structure must today be modified to improve their solubility (potentially compromising those chemical features that are responsible for their desired pharmacological effect) could be used without those changes by using nanoparticle delivery instead of chemical dissolution.

Furthermore, most drugs are delivered throughout the body, rather than to the specific area where they are meant to have an effect. As a result, side effects on other tissues are unavoidable. Nanoparticles are showing promise for the delivery of drugs to specific tissues (e.g., a tumor) where they are needed. By directing drugs primarily to their desired sites of action, lower overall doses of drugs will be given because these will concentrate where they are needed and exposure of other body tissues to the drugs will be reduced. This, in turn, will reduce undesirable side effects of the drugs.

In gene therapy, specific targeting by nanoparticle design will be extremely useful. Some current attempts at gene therapy use viral particles to aim therapy at a particular type of cell and, once there, at the appropriate location within the cell, in order for the gene therapy to have its desired effect. To date, however, the effectiveness of using viral vectors to introduce DNA into cells is quite variable. Nanoparticles may be able to deliver nucleic acids to specific cells and even to the specific compartment (cytoplasm or nucleus) within those cells — wherever their action is required.

Agency Participation and Partnerships

NIH in collaboration with other agencies, including NSF, DOD and NASA.

Examples: Even though many of the ultimate uses of nanotechnology for medicine cannot be predicted, NIH envisions some near-term (five-to-ten years from realization) applications. These include sensors for the early detection of disease, materials and strategies for dispensing therapeutic agents in ways that enhance desired effects while minimizing adverse side effects, new materials to repair and replace parts of the body damaged by age and disease, and increasingly sensitive and novel measuring tools to study biomolecular systems in their native states. To stimulate investigators to develop new research programs in nanotechnology, NIH will have announcements for the SBIR mechanism and existing grant programs under which nanotechnology research projects may be supported. In particular, the Bioengineering Research Partnerships program, organized by the NIH Bioengineering Consortium (BECON) with broad participation by the NIH Institutes and Centers, offers the opportunity for investigators from diverse scientific, clinical and engineering fields, in academia, national laboratories, and industry, to assemble the interdisciplinary teams required for much of this research.

The challenge of ensuring astronaut health and performance, drives NASA to a focus on biochemical signatures of incipient problems, and on nanoscale in vivo, and minimally invasive biochemical sensors and therapy effectors in the context of: early detection of incipient health and performance problems of astronauts; targeting and delivery of preventative and curative therapeutics; in situ detection and characterization of life beyond Earth's biosphere. NIH will collaborate with NASA in this area, and a joint program is being planned with NIH/NCI in the general area of detection and imaging at the molecular level.

There is also synergy with biosensor development outside of the medical arena in DOD and DOE covered under the Bio-Nanosensor category.

Nanoscale Processes for Environmental Improvement

<u>Vision and Strategy</u>

Vision

Nanoscience and engineering could significantly affect molecular understanding of nanoscale processes that take place in the environment; of the generation and remediation of environmental problems through control of emissions from a wide range of sources; of the development of new, "green" technologies that minimize the production of undesirable by-products; and of the remediation of existing waste sites and streams. Removal of the smallest contaminants from water supplies (less than 200 nm) and contaminated air (under 20 nm) and continuous measurement and mitigation of pollution in large areas of the environment will be achieved.

Other Grand Challenges related to energy, materials, electronic, and biodevices address the environmental technologies needed to reduce the pollution at its source.

Special Research Opportunities

Physical and chemical processes involving nanoscale structures are essential to phenomena that govern the trapping and release of nutrients and contaminants in nature. The aerosol and colloidal structures provide sites for complicated interactions with microbes that control or mediate the bioavailability of a wide variety of organic and inorganic compounds. Nanoparticles have large and active lateral surfaces that can absorb and transport pollutants in the form of colloidal suspensions and aerosols. Also, such particles are involved in complex chemical processes in the atmosphere and in soils, and can catalyze adverse reactions. An increased knowledge of the dynamics of processes specific to nanoscale structures in natural systems can improve understanding of complex processes occurring in the environment and can lead to the development of approaches for mitigating environmental harm.

In order to understand the environmental consequences of processing and transporting contaminants in the environment, interdisciplinary research is needed on molecular and nanoscale processes that take place at one or more of the interfaces or within nanoscale structures in natural systems. Such research includes studies of the interfaces between inorganic/inorganic, inorganic/organic, and organic/organic structures focused on the specific processes characterized by small-length scale.

Interdisciplinary research that involves novel approaches and that adapts newly developed experimental, theoretical, and computational methods for characterizing nanostructures is needed. The intention is to bring the community of scientists and engineers studying the fundamental properties of nanostructures together with the community attempting to understand complex processes in the environment in order to hasten the integrated understanding of the environmental role of nanoscale phenomena. Model nanostructures can be studied, but in all cases the research must be justified by its connection to naturally occurring systems or to environmentally beneficial uses. Environments for investigations are not limited and might include terrestrial locations such as acid mines, subsurface aquifers, or polar environments.

Priorities

- Study of the effects of finite size, reduced dimensions, or special geometrical arrangements of atoms or molecules on the interaction of nanoscale particles with substrates
- Development of an understanding of how structures peculiar to surfaces or interfaces influence environmentally relevant reactions
- Use of modern experimental techniques such as optical traps, laser tweezers, or synchrotron radiation to examine model environmental processes that occur within nanoparticles or at surface nanostructures
- Study of the role of nanostructures in important processes such as protein precipitation, desorption of pollutants, stability of colloidal dispersion, micelle aggregation, or microbe mobility
- Development of experimental, theoretical, and computational techniques to examine the role of nanoparticles in atmospheric and water resources processes
- Meso-porous structures integrated with micromachined components that are used to produce high-sensitivity and highly selective chip-based detectors of pollutants

Agency Participation and Partnerships:

DOE, NSF and other collaborating agencies.

Example: NSF's research in this area will focus on probing nanostructures and processes of relevance in the environment from the Earth's core to the upper atmosphere and beyond. Emphasis will be on understanding the distribution, composition, origin, and behavior of nanoscale structures under a wide variety of naturally occurring physical/chemical conditions, including nanoscale interactions at the interface between organic and inorganic solids, liquid and gases, and between living and non-living systems. This research area also includes biomineralization of nanoscale structures, development of environmental biotechnology, study of transport of ultrafine colloidal particles and aerosols, and study of interplanetary dust particles. Examples of possible applications include better understanding of molecular processes in the environment, the development of manufacturing processes that reduce pollution, and new water purification techniques and artificial photosynthetic processes for clean energy.

Efficient Energy Conversion and Storage

Vision and Strategy

Vision

Nanoscale synthesis and assembly methods will result in more energy-efficient lighting, stronger light-weight materials that will improve efficiency in transportation, use of low-energy chemical pathways to break down toxic substances for environmental remediation and restoration, better sensors and controls to increase efficiency in processing and manufacturing, and significant improvements in solar energy conversion and storage. The efficiency of solar energy conversion and of fuel cells is expected to double.

Special Research Opportunities

A key challenge is to understand how deliberate tailoring of materials at the nanoscale can lead to novel and enhanced functionalities of relevance in energy conversion, storage and conservation.

The enhanced properties of nanocrystals for novel catalysts, tailored light emission and propagation, and supercapacitors for energy storage are being explored, as are nanocomposite structures for chemical separations, adaptive/responsive behavior and impurity. Nanocrystals and layered structures offer unique opportunities for tailoring the optical, magnetic, electronic, mechanical and chemical properties of materials.

Relevance and Research Priorities

This work has significant potential for energy technologies. For example, nanocrystalline semiconductors in the form of fractal films of particles, isolated colloidal quantum dots, ordered and disordered arrays of close–packed colloidal quantum dots, and two–and three–dimensional arrays of self–organized epitaxially grown quantum dots have many potential and existing applications in renewable energy systems. These include very inexpensive and color tunable (from clear to colored to black) photovoltaic solar cells based on the dye–sensitization of nanocrystalline wide bandgap oxides (like TiO_2) operating in a photoelectrochemical cell, and novel solar cells with extremely high conversion efficiency. Nanocrystals could also be used as efficient photocatalysts for photodetoxification of polluted or toxic water and air streams. Semiconductor nanocrystals and nanostructures may be used as efficient photoactive materials for solar–photon conversion of simple molecules to fuels and chemicals, for instance photolytic water splitting to produce hydrogen, photoreduction of carbon dioxide to alcohol and hydrocarbon fuels, and photoreduction of molecular nitrogen to ammonia for fertilizer production.

A deeper understanding of the physics of phonon transport in nanostructured materials may facilitate production of practical all–solid–state and environmentally clean thermoelectric energy–conversion devices with performances far superior to current vapor–based refrigerators and combustion–based engines. The pervasive role of hard and soft magnets in electric–power production and utilization is another arena in which new nanoscale magnetic materials may yield substantial energy savings by reducing losses and conserving natural resources consumed in the generation and use of electricity.

Nanostructured carbon–based nanotubes have the potential to act as a hydrogen storage medium that could exhibit very high storage density per unit weight, which is critical for hydrogen–based transportation systems. A crucial issue is whether or not the hydrogen could be extracted efficiently from such a storage medium at relatively low temperatures.

Opportunities exist for increasing thermal transport rates in fluids by suspending nanocrystalline particles in them. These "nanofluids" have recently been shown to exhibit substantially increased thermal conductivities and heat transfer rates compared to fluids that do not contain suspended particles. However, there is no real understanding of the mechanisms by which nanoparticles alter thermal transport in liquids. Multibillion–dollar industries, including transportation, energy, electronics, textiles, and paper, employ heat exchangers that require fluids for efficient heat transfer. If researchers can improve these fluids, there can be significant gains in efficiency.

Nanostructured materials also promise greatly improved structural properties in comparison with conventional metal alloys. For example, small–diameter bundles of single–walled carbon nanotubes are predicted and observed to have the largest strength–to–weight ratio of any known material, which is approximately *one hundred times that of steel but with only one–sixth its weight*.

Such materials offer opportunities for reducing the weight of automobiles and increasing fuel economy, if they can made by an economically competitive process that is compatible with other manufacturing technologies.

Other examples of new or enhanced properties from nanostructured materials that can improve energy technologies include:

- Nanoscale layered materials that can yield a four-fold increase in the performance of permanent magnets
- Addition of aluminum oxide nanoparticles that converts aluminum metal into a material with wear resistance equal to that of the best bearing steel
- Layered quantum well structures to produce highly efficient, low-power light sources and photovoltaic cells
- Novel chemical properties of nanocrystals that show promise as photocatalysts for more energy efficient breakdown of toxic wastes
- Meso-porous inorganic hosts with self-assembled organic monolayers that are used to trap and remove heavy metals from the environment

While microsystems and microdevices are built on the dimensional scale of microns to centimeters, their functionality and performance depend on the understanding and control of materials properties on the nanoscale. Some of the nanoscale science and technology issues that are relevant for micro-electro-mechanical devices are lubrication, friction, wear, and micro-mechanical properties. Examples of current research include the science of self-assembled nanolayers to reduce adhesion and friction, and the development and use of new interfacial force microscopies to study lubrication at the nanoscale. Areas of interest in the area of micro-electro-mechanical devices include an understanding of materials performance and aging under operational conditions, including mechanical stresses and atmospheric environments; methods of surface preparation/passivation/ lubrication for the purpose of minimizing adhesion, friction, wear and corrosion; novel analytical techniques and diagnostics to probe performance and degradation phenomena at molecular size scales (particularly spatially resolved techniques), polymer or other silicon-compatible optical components and sensors; studies to relate operating lifetime of the integrated microsystems, and any of their component nanotechnologies, to details of the fabrication process, and investigations of the operation of these systems in extreme environments, including shock, vibration, extreme temperature excursions and radiation. Investigations of these phenomena with nanostructures holds the promise for understanding the initiation mechanisms of friction, wear, fatigue and other causes of materials failure.

Research Priorities

- For future generations of energy systems, nanotechnology can provide significant advances in terms of functionality, speed and capacity.
- Innovative approaches to improved conversion of solar energy into electricity.
- Catalysts for improved conversion of hydrocarbon energy into thermal energy; Catalysts and membranes that enable effective, commercially viable fuel cells that utilize a range of materials as fuels.
- Nanostructured materials for thermoelectricity, magnetic refrigeration and other innovations in efficient energy conversion.

- Improved materials and coatings for reduced materials failure rates and lower friction (wasted energy dissipation)
- Nanostructures that will selectively bind and concentrate radionucleotides, thereby sequestering them from benign waste material and lowering waste disposal costs for nuclear energy.
- Nanostructured materials that are more radiation tolerant for greater nuclear reactor lifetimes.
- Advances in nanoelectronics development could enable new generations of high speed, low power circuits for special purpose high performance needs.

<u>Agency Participation and Partnerships</u>

DOE and other collaborating agencies including DOC, NSF, NASA and DOD.

Example of partnership: NASA will collaborate with DOE, DOD and NSF for high-efficiency, low mass solar and thermal energy conversion for space power, high-mass-efficiency power storage and distribution, and efficient low-temperature refrigeration for ultra-sensitive space-based sensors. NASA has an ongoing program with Rice University with a focus on applications of carbon nanotubes to aerospace vehicle structures, batteries and energy storage, and nano devices. A number of other universities are involved in various aspects of the ongoing nanotechnology work.

Microcraft Space Exploration and Industrialization

<u>Vision and Strategy</u>

Vision

Continuous presence in space outside of the solar system with nanotechnology enabled low powered microspacecraft. Reduce the size and energy consumption ten fold.

Special Research Opportunities

Microspacecraft development is a key thrust for the exploration of space. Motivators for this demand include the high cost of launching into space, the desire to reach ever more remote and hostile environments in our solar system, and the unique capabilities of missions involving large numbers of cooperative spacecraft. To fulfill the promise that microspacecraft hold for exploring space, these spacecraft cannot be scaled down versions of larger spacecraft, limited in capability. This new breed of spacecraft must surpass the current state of technology in today's fleets of vehicles. Long duration missions (decades) to the outer reaches of the solar system; exploration into the interiors of planets, comets, and moons, searching for the subtle clues of the presence of life; fleets of telescopes, acting in concert, imaging Earthly planets around other stars; all these long range goals for space exploration in the 21st century will be enabled through the development of advanced nanoscale technology.

Priorities

The key challenge for NASA is identifying, developing, and exploiting nanotechnology advances that offer unique advantages for space exploration. Research areas that are promising in achieving the nation's space goals include:

1. *Nanostructured materials*: one key enabling technology for future NASA missions is the development of ultralight weight and ultrastrong materials that can survive the space environment. These materials are necessary for the creation of very large structures (telescopes, antennas, solar sails, to name a few) whose mass will be a only a small fraction of current systems. The utilization of these materials in deployable and inflatable systems permits very small spacecraft to undertake missions that were otherwise deemed far too costly or simply undoable. Beyond the mass and strength advantages of nanoscale materials lie unique optical, piezoelectric, and other material properties that will allow the creation of truly smart and agile structures. Active control of mirror surfaces, adjustable thermal properties, and self-repairing materials represent a partial list of developments that will change how space missions will be done.

2. *Nanoelectronics*: Processing, sensing and information management technologies are critical for space systems. Strong pushes for much more capable spacecraft electronics come from the following:
   - greater autonomy and on board decision making,
   - the large, diverse data sets to be collected by future missions,
   - greater sensitivities of the scientific instruments,
   - Sophisticated fault management and self-repair capability.
   - However, these requirements are colliding with the realities of the limitations of microelectronics, with space applications putting extreme demands on the electronics for ultralow power consumption, radiation tolerance, and safety. The development of transistors and other circuit elements utilizing single quantum excitations (electrons, Cooper pairs, photons) enable spacecraft to collect, process and then transmit information that will far surpass the capabilities of current missions. Specific examples include:
   - detectors capable of detecting and measuring single photons, which will fully utilize the large area apertures enabled by nanoscale materials
   - non volatile, radiation resistant, high density memory systems
   - ultrahigh speed computation, for s/c decision making and data set reduction
   - rugged, miniaturized spacecraft avionics systems utilizing microwatts of power

3. *Biomimetic systems*: Micro systems based on biological principles, or on biological building blocks, is a key future area for space exploration. Ultra long duration missions, or missions in hazardous environments, will benefit greatly from adopting strategies and architectures from the biological world. Also, in the search for life outside the earth, understanding and controlling processes at the molecular level is necessary for enabling in situ systems to carry out advanced laboratory analyses. Self replicating systems, utilization of in situ resources to create complex structures in space, spacecraft that can adapt and react to changing environmental or mission needs are examples of the kinds of advances that NASA is pushing to be enabled through applying nanotechnology and molecular biology methods to spacecraft.

Agency Participation and Partnerships

NASA and other collaborating agencies including DOD, DARPA, NSF, and NIH/NCI. *NASA expects to allocate the majority (50-60%) of its nanotechnology program funds to address priority challenges of future robotic and human aerospace systems.*

Example: NASA's focus in this area is on low-mass, low-power, devices, subsystems and systems with goals of: reduction in size and energy consumption of capable spacecraft by a factor of 10; greatly increased on-board capability for signal processing, real-time decision making and autonomy; low-power, miniature spacecraft systems including sensors, signal processing, avionics, inertial guidance, propulsion and communications; Earth-to-orbit and deep-space transportation based on more reliable materials and smart systems for condition-based maintenance; bio-mimetic evolvable space system architectures that can adapt to new environments and mission needs, and eventually to self-replicate using local resources at distant locations. DOD is an agency with overlapping interests (low-cost air and space transportation). DOD and NASA will cooperate in developing microspacecraft.

Bio-nanosensor Devices for Communicable Disease and Biological Threat Detection

<u>Vision and Strategy</u>

Vision
Nanoscience and technology will foster efficient and rapid biochemical detection and mitigation in situ for chemical-biowarfare, HIV, and tuberculosis. Miniaturized electrical/mechanical/chemical devices will extend human performance, protect health, and repair cellular/tissue damage.

Special Research Opportunities
Minimally intrusive devices for human tissue and vasculature will benefit from nanoscale manufacturing. As the structures are reduced to nanometer scale size, molecular structures will begin to compete with inorganic structures, and new device functions will be made possible. The opportunities for molecular mechanical systems are compelling. Living systems depend on a variety of molecular motors. Molecular motors derive their power from body chemistry; it is possible that an *in vivo* bionanodevice could be powered by that same body chemistry.
For *ex situ* applications, the bionanodevices must be able to sense and identify pathogenic chemical/biological species and then initiate action to neutralize the pathogen. Most chemical/biological detectors select for a known threat. It is important to develop detectors that can sense distress in living cell/tissue and alarm the organism to the presence of an unknown threat. Such a detector will require attention to interactions between inanimate silicon devices and living organic devices. Microfluidics, wall adsorption, fouling will be critical issues for attention. Nanometer-sized clusters can have novel properties and can provide new approaches to the difficult problem of species neutralization without hazard to personnel and machinery. *Ex situ* size constraints will be less severe on Bionanodevices. This application will be a stepping stone toward *in situ* application.

As *in vivo* systems, bionanodevices will initiate appropriate biochemical and biophysical responses by stimulating biomolecular systems. Highly specific, functional biomolecules — poly-nucleic, peptide, and saccharide — can be synthesized by chemical/biological techniques. These molecules hold promise as highly selective sensors (DNA pairing, antibody and antigen, receptor recognition) and actuators (molecular motors from flagella and muscle, ion channel activation) to interact with body chemistry and physics. This Grand Challenge will require those biomolecules to be isolated, their structure and properties relationships understood, their coupling to inorganic substrates without loss of function determined, the mechanisms for communication between biomolecules and

semiconductor electronics ascertained, and the extent of power that can be derived from body chemistry ascertained. Better techniques for single molecule manipulation and measurement must be developed using proximal probes and optical tweezers.

Relevance

Miniaturized, low power, sensitive, and selective detection/remediation of biological and chemical threats is a recognized problem with immediate significance because of concern over weapons of mass destruction. Mother Nature has produced some of the worst threats to humans — HIV, TB, and the Ebola virus, to name a few. Public health, military and police forces are in desperate need of the improvements expected from bionanodevices. These sensors will revolutionize medical diagnostics, making sophisticated blood/urine/saliva tests inexpensive and routine operations at the doctor's office. Many professions require sustained human performance under demanding conditions — pilots, the military, police — even so simple a task as long-distance driving. Bionanodevices will monitor body chemistry and physics, provide alerts to mental or physical deterioration, and take appropriate countermeasures. As miniaturization progresses, bionanodevices will be inserted into the body with the ability to recognize locations in distress (like cancer sites, infections, calcification, and bleeding) and take localized, measured remedial action. Whole body infusion of a prophylactic drug won't be necessary. Cancerous tissue can be treated directly without disturbing healthy tissue. In addition to general health care, the casualty care of special concern to police, trauma, and military operations will benefit.

Priorities and Modes of Support

- Development and measurement of single supramolecular chemical, biological, and physical properties
- Development of nanomechanical systems, miniaturization of micoelectromechanical systems (MEMS) by a thousand-fold, and incorporation of molecular activation and motility
- Sense and actuate information transfer between inorganic electronics and biomolecular systems

Infrastructure

Bionanodevices will require extremely close coupling among various disciplines, especially biology and the physical/engineering sciences and the microelectronics communities. Centers facilitating such interaction will be essential. The fabrication of nanometer-sized electromechanical devices will need the equivalent of the Microelectronics Center of North Carolina's Multi-User MEMS Processes (MUMPS) facility that presently enables affordable manufacture of MEMS devices for research purposes.

<u>Agency Participation and Partnerships</u>

NSF, NIH, DOD and DOE. *NSF will invest in fundamental science base.*

Examples: NIH will focus on bionanotechnology approaches to body chemistry intervention. DOD will focus on development of nanoelectromechanical systems (NEMS) and chemical-bio agent detection. DOE will contribute with laboratory on a chip concepts. NASA's focus in this area is on nanoscale sensors and integrated laboratories for the purpose of monitoring and controlling human space habitat environments. Agencies with overlapping interests are DOD (detection of biochem-warfare agents), DOE (lab-on-a-chip for detecting environmental pollutants and biological threats).

Application to Economical and Safe Transportation

Vision and Strategy

Vision

Nanotechnology will be the building tool for advances in transportation in the 21st century. It's potential benefits are broad and pervasive, including lighter and more efficient cars using nanostructured materials, corrosion-free bridges and no-maintenance roads, and tiny "traps" that remove pollutants from vehicle emissions.

Among the **breakthrough applications** that we may see in transportation are the following:

- Nanotechnology will yield advanced materials that will allow for longer service life and lower failure rates. Among the key applications are: nanocoating of metallic surfaces to achieve super-hardening, low friction, and enhanced corrosion protection; "tailored" materials for infrastructure and vehicles; and "smart" materials that monitor and assess their own status and health and repair any defects including fire-resistant materials in vehicles and aircraft.
- Applications of nanoelectronics for transportation include: advanced communications that maximize the benefits of intelligent transportation systems and obviate the need for some travel altogether; sensors that continuously monitor the condition and performance of roads, bridges, and other infrastructure; and "brilliant" vehicles that can avoid crashes and improve operator performance.
- New materials developed through nanotechnology will permit the ultra-miniaturization of space systems and equipment, including the development of smart, compact sensors; miniscule probes; and microspacecraft. Applications include: economical supersonic aircraft; low-power, radiation-hard computing systems for autonomous space vehicles; and advanced aircraft avionics.
- Nanotechnology has the potential to reduce transportation energy use and its impacts on the environment. Applications include nanosensors used to monitor vehicle emissions and to trap any pollutants; nanoparticle-reinforced materials that replace metallic components in cars; replacement of carbon black in tires with nanoparticles of inorganic clays and polymers, leading to tires that are environmentally friendly and wear-resistant; and carbon-based nanostructures that serve as "hydrogen supersponges" in vehicle fuel cells.

Agency Participation and Partnerships

Various agencies, including DOE, DOD, NIST and NASA, are developing materials and manufacturing technologies for transportation.

For example, DOE's contribution will be primarily in energy storage (e.g., hydrogen); emissions reduction (e.g., traps); and materials for vehicles. In addition, DOT will leverage other agencies' efforts through (1) support for a broad program of university research and education in nanotechnology; and (2) targeted research programs to expedite the development of promising applications for highway, rail, and air transportation.

National Security

Vision and Strategy

Vision
Retain and extend technology to enable rapid military dominance simultaneously with reduced manpower, lower human exposure to risk, and more affordable systems. DOD and DOE investment in nanoscience is essential to meet their stated goals of knowledge superiority, full spectrum dominance, warrior protection and a highly secure, extended-life nuclear stockpile in the 21st century.

Relevance
The 1998 Defense Science Board study "Joint Operations Superiority in the 21st Century" states that: "Perhaps the most pervasive operational challenge enabling early and continuous combat effectiveness is knowledge superiority**.**" Nanoscience and technology will enable us to achieve knowledge superiority at all levels, in the 2020 time frame. It can lead to incredible gains: in sensor suites with 1000 times smaller size/power embedded in autonomous microsystems; in processors with 100 times faster speed, 100 times higher density, and 1000 times less power per function; in nonvolatile, radiation-resistant static memory with 100 times higher density and 50 times faster access speed; in flat, foldable displays with 10 times greater brightness (nanophosphors) without a concomitant increase in power requirements; and in communications with 100 times greater bandwidth. The Network Centric Warfare, Information Warfare, and Simulation/Modeling operations — already accelerated by the previous improvements in information technology hardware — will be revolutionized once again through these additional breakthroughs in hardware capability.

The new capability will include worldwide, instantaneous communication, threat identification, secure encryption, speech recognition/language translation for joint operations, and combat ID. The huge data streams from multispectral imaging (visible, infrared, mm-wave, microwave, and acoustic) will be transmitted, processed, correlated, and presented in millisecond time frames. The enhancements will enable the service goals of smarter weapons for surgical strikes and uninhabited combat vehicles, with special value for aircraft whose agility will improve significantly without human g-force limitations. The automation stemming from greater information processing coupled with nanofabricated sensing suites and nanoelectromechanical actuation will result in a reduced workforce. The greater training requirements imposed by the reduction in manpower will be met by affordable personal virtual reality trainers. The realization of these new concepts will require all these advances in sensing/processing/storage/display transmission.

The central theme of Joint Vision 2010 is full spectrum dominance, including dominant maneuver, precision engagement and full dimensional protection. These requirements translate into high performance platforms — satellite, aircraft, surface ship, submarine, armored vehicle — all needing premiere materials at affordable costs. Nanostructures have novel properties not otherwise available. Their small size also permits their selective incorporation into composites with tailored performance characteristics. Expected improvements include the following: reduced manufacturing costs by self-assembly of smaller units into larger structures rather than costly machining down from bulk and by net-shape formation of ceramics through novel nanostructure interface mechanics;

organic composites with high strength-to-weight made by including nanotubes (whose measured strengths are among the highest known) or with fire resistance created by including nanoclays (enabling the use of organic composites in surface ships and submarines); multispectral (visible, infrared, mm-wave, microwave, acoustic) low observable materials made by incorporating quantum dots and nanocrystal networks; lowered maintenance costs by nanostructured coatings with reduced wear/corrosion/thermal transport; higher efficiency energy conversion technology with nanostructured fuel cells, solar cells, and batteries; and smart materials that detect and respond to the environment through embedded nanosensors and nanoactuators (e.g., to sense a sonar or radar ping and squelch any echo).

Defense ultimately relies on the warrior; information and platforms are aids, not ends. We must protect the warrior from weapons of mass destruction; sense and aid his performance, especially under the extreme operating demands placed on him; and provides the casualty care he deserves. Bionanodevices will revolutionize these capabilities. The techniques and tools of nanoscience will detect single pathogens, providing the ultimate in sensitivity for chemical and biological agents packaged in fast, low-power, affordable systems no bigger than badges. Nanostructures show promise for the catalytic degradation of pathogens/chemical agents with less damage to the environment. The marriage of nanoelectronics with molecular biology will enable in-situ, body powered sensors (for pathogens, alertness, fatigue) with the ability to take action to protect the individual or enhance his performance (augmented sensory capability — hearing, vision, smell, touch).

For the nuclear stockpile, the potential of nanoscale science will be realized in weapon microsystem components for increased safety, security, and reliability in physics experiments for targets and diagnostics and in weapons surveillance. In addition, science at the nanoscale is required for first-principles, high-fidelity models and simulations to predict the performance and lifetimes of weapons systems.

Priorities

The DOD Basic Research Plan has designated a Special Research Area — Nanoscience — with the following goal: "to achieve dramatic, innovative enhancements in the properties and performance of structures, materials, and devices that have ultra-small — but controllable — features on the nanoscale.…" In the last fifty years, DOD funding has been a principal federal source of research support for the next generation of electronic/optoelectronic devices, affordable, high performance materials, and defense against weapons of mass destruction. The pending DOD-relevant nanotechnology investment has several common objectives with other Grand Challenges addressed to civilian use:

- The priorities in nanoelectronics/optoelectronics are as follows:
- Synthesis/processing of quality nanostructures that can translate to commercially affordable processing technology: self-assembly, parallel processing via proximal probes, and in-situ processing controls
- Measurement of nanostructure properties: quantum effects, tunneling, exchange coupling, molecular electron transport, and terahertz response
- Innovative device concepts: single electron devices, spin-electronics, quantum dots, and molecular electronics

- Potential system architectures: cellular automata, quantum computers, cellular parallel computers, and multiple function integration
- Modeling/simulation for accelerated device/system progress
- Advanced optical components: photonic crystals, and novel phosphors
- Autonomous microsystems coupling sensing, processing, storage, actuation, communication, and the power to facilitate a complete tactical picture

The priorities in affordable, high-performance nanostructured materials are as follows:

- High volume manufacture of high quality clusters, nanotubes, and dendrimers
- New materials fabrication paradigms: superplasticity and self-assembly
- Formation and properties of high surface area materials, nanocrystal networks, and aerogels
- Measurement of individual nanostructure properties and of the interfacial properties in nanostructured materials
- Physics of the nanometer-scale initiation events of materials failure
- Tailored coatings for affordability — wear, corrosion, thermal barrier, and energy harvesting
- Smart materials for condition based maintenance, and for low observable signatures
- Models/simulations incorporating multi-scale (atomic to nanostructure to microstructure to macroscopic) computation and leading to materials by design

The priorities in bionanodevices are as follows:

- Measurements of single supramolecular properties to define the events of molecular recognition and dynamics
- Design and implement molecules to interface between nanodevices and body chemistry
- Nanoelectromechanical systems (NEMS), especially utilizing molecular motors as potential actuators

DOE investments focus on performance, diagnostics and long-term aging elements of the nuclear stockpile which promise to be revolutionized by advances in nanoscale science. A life-extended stockpile with the needed safety and security enhancements within current system and space constraints will also draw upon nanoelectronic, nanooptic, and nanoscale materials advances. This control at the nanoscale will enable, for example, the introduction of microsystems with the needed performance, size, and lifetimes to meet future needs of stockpile refurbishment.

Agency Participation and Partnerships

DOD and DOE in partnership with NSF and NIH.

Examples: The DOD programs in nanoelectronics/electrooptics and materials are in partnership with NSF Centers, DOE facilities, and industry. The DOD expects to build on NIH investment in bionanodevices, focusing the vast opportunities there on specific DOD needs. A more detailed portrayal of the role of nanoscience and nanotechnology in DOE Defense Programs Research is given in the white paper 'DOE Defense Programs Research in Nanosciences: Predictive Understanding and New Materials Concepts'.

11. <u>Centers and Networks of Excellence</u>

(total FY 2001 is $77 million, $30 million above FY 2000)

<u>Vision and Strategy</u>

Vision

Fund ten nanoscience and technology centers and networks at about $3 million/year for approximately five years with opportunity of one renewal after the review. A focus on research networking and shared academic user facilities is recommended. The establishment of nanoscience and technology research centers similar to the supercomputer centers will play a critical role in attaining other initiative priorities (fundamental research, Grand Challenges, and education), development and utilization of the specific tools, and in promoting partnerships. Collaboration with academic networks (such as NNUN for nanotechnology equipment and DesCArtES for nanoelectronics software), and with national users facilities (such as synchrotron radiation facilities and neutron sources at national laboratories) is envisioned.

Special Opportunities

The science of nanostructures has become a theme common to many disciplines, from nanoelectronics and molecular biology to catalysis, filtration and materials science. Each of these disciplines has evolved its own independent view of nanoscience; the opportunity to integrate these views and to share the tools and techniques developed separately by each field, is one of the most exciting in all of science and brings with it enormous potential for technological innovation. Centers for nanoscience and technology will be a major component of the spectrum of support for this increasingly interdisciplinary field, with potential impact beyond that of single investigator programs.

A related need is for adequate advanced facilities to do the research demanded by nanoscience and technology. As George Whitesides and Paul Alivisatos have pointed out, to make rabbit stew, you must first catch a rabbit. In order to work in nanoscience, one must be able to fabricate and characterize nanostructures. In many cases the requisite fabrication and characterization facilities are beyond the scope of individual-investigator laboratories – it takes the scope and infrastructure of a center or 'shared facility' to equip and maintain them. Access to sophisticated and well-maintained facilities and instrumentation together with support for instrument development will be essential to the success of research and education nanoscience and technology.

The proposed centers will be critical to support and accomplish the core objectives of the initiative: interdisciplinary fundamental research (budget request for FY 2001: $40 million, a $15M/yr increase over FY 2000), Grand Challenges ($20 million, a $8M/yr increase), laboratory infrastructure ($17 million, a $7M/yr increase), and education and training.

Priorities and Modes of Support

Nanoscience and Technology Centers and Networks (NTCs) will catalyze the integration of research and education in nanoscience and technology across disciplines and among sectors including universities, government laboratories and the private sector. They will also help to provide the sophisticated tools needed to do the work.. NSF's Science and Technology Centers (STCs), Engineering Research Centers (ERCs), and Materials Research Science and Engineering Centers (MRSECs) provide successful models for this process over a very wide range of science

and engineering. DOD's Multidisciplinary University Research Initiative (MURI), and DOE's and NASA's university-based research centers provide successful patterns for mission oriented centers. The NTCs will include partnership among academic institutions and between academia, government laboratories and the private sector as needed. They will address interdisciplinary areas such as simulation at the nanoscale, device and systems architecture at the nanoscale, nanomaterials, nanoscale structures and quantum control, nanofabrication, hierarchical linking across multiple length and complexity scales, nanotechnology and biorobotics, nature and bio-inspired materials and systems, nanoscience for health care, and molecular nanostructures.

NTCs will:

- Address major fundamental problems in nanoscience and technology, bringing to bear the entire spectrum of disciplines including engineering, mathematics and computer science, physical sciences, earth science, and biological and medical sciences as needed. Exploratory research and vertical integration from fundamental research to innovative technological outcomes will be encouraged. Stimulate and support interagency partnerships to foster emerging areas of nanoscience and technology at interdisciplinary frontiers.
- Support interdisciplinary research groups comprising strongly coupled groups of investigators - the whole must be greater than the sum of the parts. Provide incentives to enable interdisciplinary research and education to prosper;
- Develop and sustain strong links between experiment, theory, modeling and simulation to advance nanoscience and engineering;
- Integrate research and education from pre-college through postdoctoral;
- Provide and maintain state of the art instrumentation and shared user facilities that are beyond the reach of benchtop science, including fabrication and characterization equipment, for the benefit of users both within and outside the centers;
- Foster intensive cooperation, collaboration and partnerships among investigators from universities, government laboratories and industry involved in nanotechnology. Programs for visitors from industry and other research centers will be established.
- Promote exchange programs for students and faculty with other centers of excellence in the US and from abroad;
- Include effective collaboration with and access to unique capabilities offered by existing facilities at such as synchrotron x-ray, neutron sources, the National High Magnetic Field Laboratory, the National Nanofabrication User Network, and advanced computational facilities and resources, through partnership with national laboratories and other institutions and centers as needed;
- Provide access to databases, remote access to instrumentation, and links from research and education to producers and users of nanotechnology;
- Allow investigators flexibility to pursue promising new lines of high-risk research within the overall scope of the Center's goals, without agency 'micromanagement.'

Infrastructure

Physical laboratory infrastructure will be created in the emerging areas of nanoscience and technology, including expensive equipment that can not be obtained or adequately maintained by individual academic researchers. This will contribute to an advanced and balanced infrastructure.

The educational value of NTCs and their role in workforce development deserves special mention. They will provide both a horizontal and vertical integration of education, with students interacting at all levels of their training: precollege, undergraduate, graduate students, postdocs, junior and senior faculty and investigators from industry and government labs. They will also provide a platform for outreach to generate and maintain public support for nanoscience and technology, and for curriculum development in critical cross-disciplinary areas involving engineering, the physical sciences and biology.

*The proposed investment for FY 2001 ($77 million, a $30 million increase) will be used to e*stablish approximately ten new nanoscience and technology centers/networks by competitive review, each at about $3M total funding over approximately 5 years, renewable for a further 5 years. Each NTC will address a major topical area in nanoscience and technology, and will support about 10-20 core researchers plus students and postdocs and support for instrumentation, access to facilities, materials and supplies, partnership with industry and national laboratories as appropriate, and programs for education and outreach. The new centers will be integrated in the existing group of about 15 large university-based and national laboratory-based centers with research on nanoscale science and engineering.

<u>Agency Participation and Partnerships</u>

All participating agencies.

Examples: NSF will focus on university-based centers and networks, while other agencies will support a combination of government research laboratories and academic institutions. Vertical integration from fundamental research to technological innovation will be supported by joint funding from NSF and mission oriented agencies, DOD, DOE, NASA and NIH, respectively. Five-ten university-based centers on simulation at nanoscale, integration at nanoscale, interaction processes at nanoscale, nanofabrication, nanotechnology and bio-robotics, and nano-biomedicine are planned by NSF, DOD and NIH. National laboratory-based research and user facilities will be operated at several government-sponsored laboratories.

NASA will offer opportunities to work with university research centers to arrange for student and postdocs' participation in NASA's grand challenge research, including opportunities to work for periods of time at NASA Centers.

NIH has in place mechanisms to support fundamental research and projects to meet grand challenges for the solution to specific biomedical problems, through individual laboratory and "centers"

12. <u>Research Infrastructure</u>

(total FY 2001 is $80 million, $30 million above FY 2000)

<u>Vision and Strategy</u>

One of the NSET "high priority" themes for additional funding beginning in FY2001 is 'research infrastructure' that includes metrology (budget request for FY 2001: $10 million, a $6 million increase over FY 2000), instrumentation ($30 million, a $8 million increase), modeling and simulation ($15 million, a $6 million increase), and user facilities ($25 million, a $10 million).

Vision
A balanced, strong, but flexible infrastructure will be developed to stimulate new discoveries and innovations that can be rapidly commercialized by U.S. industry. The focus will be on developing measurements and standards, research instrumentation, modeling and simulation capabilities, and R&D user facilities.

The potential is great for universities and government to transition this science and technology, bringing forth fundamental changes. There are great demands in industry to attract new ideas, protect intellectual property, and develop high performance products. The transition will require a sustained and timely investment. If the issues associated with research infrastructure and transition from knowledge-driven to product-driven efforts are not satisfactorily addressed, the United States will not remain internationally competitive and, therefore, have difficulty maintaining the economy and quality of life and security that exist today.

Metrology (Measurement Technology)

Challenges and Opportunities
Nanotechnology offers an outstanding challenge to measurement technology by requiring three-dimensional, atomic-scale measurement capabilities over large areas. To design, observe, test, and understand the next generation of nanodevices, we must be able to measure all the important physical, chemical and at times biological parameters associated with the devices. These measurements are not currently possible because the necessary tools and theories are only rudimentary, but must be developed through this Federal Initiative. .

While nanoscale measurement is challenging, nanotechnology offers totally new mechanisms and instruments for measurements of new phenomena at subatomic spatial scales. Those measurements are currently out of our reach. Also, exquisitely accurate measurements of macroscopic physical, chemical and biological properties are possible through nanotechnology.
Priorities
The research supported by this federal nanotechnology initiative will:
- Develop new measurement systems with intrinsic, atomic-scale accuracy for length, mass, chemical composition, electricity, magnetism and other properties;
- Develop a fundamental understanding of the interactions of matter at the single atom, and molecule level allowing the design of new measurement approaches and instruments; and
- Create new standard materials, standard data, analytical methods, and standard tools to assure the quality of the new nano-based commercial products.
- Rapid transfer of the new measuring techniques and standards to industry.

The new measurement capabilities developed through this initiative will impact all industrial sectors and the everyday lives of each American. For example, new health related measurements will improve the accuracy, availability, and cost of diagnostic tests and allow more diseases to be diagnosed in a timely fashion. The reliability, cost, and function of cars, planes, telephones, computers and many other devices will improve through manufacturing improvements enabled by these measurements. For example, nanometer accuracy has made possible the giant magnetoresistance layers to be manufactured and the most advanced NASA spacecraft to be built.

Agency Participation and Partnerships

DOC/NIST will collaborate with other agencies as a function of the area of relevance. NIST will develop the critical enabling infrastructural measurement, standards and data in the areas of nanodevices, nanomagnetics, nanomanipulation, and nanocharacterization.

Example: As nanotechnology is a broad field with diverse industry needs, NIST will leverage efforts to efficiently and effectively meet the measurement and standards needs of U.S. industry while maintaining institutional flexibility and responsiveness to rapidly changing customer needs. NIST will develop stronger strategic alliances/collaborations with universities, businesses and other government agencies that possess leading expertise in nanotechnology to conduct the specific work required to meet the goals of this initiative and avoid developing costly, complex in-house capabilities that will be used only once. The university alliances will also help educate the U.S. workforce in nanotechnology-related problems, and permit NIST scientists and engineers to concentrate on the critically needed metrology and research, while contracting out development of specific equipment and techniques. Building these partnerships will return greater value to the taxpayers for their investment in nanotechnology. Table V illustrates main NNI activities to be undertaken by NIST in FY 2001. It is estimated that nanotechnology will have a major effect on every industrial sector, and will require a large infrastructure to aid rapid U.S. commercialization of new discoveries. A major portion of that infrastructure is government laboratories and particularly NIST-based measurements, standards and data that industry must use to see if and how well their products work.

Table V. Main FY 2001 NNI activities at NIST

Nanodevices	• Develop two new standard reference materials for semiconductor, lab-on-a-chip, and other nanotechnologies • Develop new quantitative measurement methods for analysis of physical and chemical properties of industrial nanoscale devices such as semiconductors • Publish reference documentation on the development of measurement methods, standard reference materials, and calibration systems.
Nanomanipulation	• Develop standards for autonomous atom assembly. • Develop modeling and simulation programs for condensed phases, including solutions, surfaces, solids, and interfaces • Publish reference documentation on the development of manipulation and modeling data, algorithms, and related research.
Nanocharacterization	• Develop three new standard reference materials for calibration and quality assurance of commercial analysis laboratories and instruments. • Develop several 3-D measurement methods for the analysis of physical and chemical at or near atomic spatial resolution. • Publish documentation on the development of measurement methods and standard reference materials.
Nanomagnetics	• Develop stability and kinetics measurement systems and standard data for magnetic thin films. • Develop two new standard reference materials. • Publish documentation and two university partnership papers per year on the measurements and standard reference materials for magnetic data storage.

Instrumentation

Challenges and Opportunities

Availability of instrumentation in university, government laboratories and industry will be a determining factor in the advancement of the field. This initiative will provide tools to investigators in nano-science and engineering to carry out state-of-the-art research, to achieve the nanotechnology potential, and to remain competitive. Funding support will include the continuous development and advancement of the instrumentation for nanotechnology in partnership with the private sector.

In the last few years there has been continually increasing interest in nanotechnology here in the United States as well as in Japan and Europe. It is critical that we have the state-of-the-art instrumentation for development of materials at the nano-scale and processing of nanostructures and devices, development of nano-scale systems, and for testing, measurements, and characterization. Progress is being made in the instrumentation - such as the scanning tunneling microscope (STM), the atomic force microscope (AFM) and near-field microscopy (NFM) - which has been developed, for the observation, characterization and analysis of nanostructures. These instruments and the development of relevant technologies are helping scientists and engineers in making scientific advances in the area of nanotechnology. At the same time these tools are being modified and improved to increase the capabilities available for manipulation and manufacturing of nanostructures.

It is possible to make nanomaterials and nanostructures using the existing facilities and capabilities available in many of the above mentioned disciplines. However, to make significant progress and impact in nanotechnology, we will have to extend those capabilities and to develop more interdisciplinary facilities that have the appropriate instrumentation.

Priorities

- Development of new instruments for research, development and processing in nanotechnology. Instrumentation for the characterization of individual and ensembled nanostructures will be required. For example, the development, detection, and manipulation of biological structures, semiconductor technology and polymeric materials will require instrumentation that is capable of handling all these materials in one facility and without the danger of cross-contamination.
- Fund the purchase of instrumentation enhancing the capabilities of the existing research centers, networks and consortiums. This includes funding of industry/university/government collaboration to develop the tools and technology. The major R&D instrumentation and facilities will be made available to users not only from the institution that houses the facilities, but also for users from other institutions, industries and government.
- Provide computer network capabilities and a nanotechnology database for the management and dissemination of information to the nanotechnology science and engineering community in order to promote collaborations.

<u>Agency Participation and Partnerships</u>

The development of the instrumentation and capabilities for research and development in nanotechnology will require cooperation and collaboration of scientists and engineers from

universities, industries, and the funding support of all government agencies. NSF, DOD, DOE and NASA will develop the instrumentation infrastructure in universities and government laboratories.

Example: Generic, broad science and engineering applications that encompass a range of hardware resources will be made possible. For NSF, the needs of the broader scientific and engineering community will drive nanotechnology infrastructure requirement in the Major Research Instrumentation and research equipment awards, emphasizing generic tools and nanofabrication infrastructure. Large-scale scientific and engineering applications that require extensive use of the hardware resources toward a focused goal. For DOE, DOD and NASA, the needs of the scientific community in the initial applications areas will drive the nanotechnology infrastructure requirements and its subsequent development.

Modeling and Simulation Infrastructure

Challenges and Opportunities

Experimentation and modeling/simulation capabilities will be equally important to advances in understanding, each testing and stimulating the other, compelling the development of new computational methods, algorithms and high performance computing resources.

Modeling and simulation at nanoscale will enable new synthesis and processing methods of nanostructures, control of nano-manipulators such as atomic force microscopes, development of scale-up techniques, and creation of complex systems and architecture based on nanostructures. Control of nano-manufacturing requires the development of manipulation strategies and associated software, using either known or new robotics techniques. Nanoassembly must be automated because the number of elementary operations required in most assemblies would be enormous. Research is needed into the programming languages suitable for assembly, into the techniques for path planning and other high-level control, and into the real-time control of singe manipulators and arrays of manipulators.

Simulation and design software will *depend upon high-speed scientific computation*. Research will be needed in information technology that creates new specialized software, algorithms, and hardware that enable more effective scientific and engineering computations at nanoscale. In particular, nanodesign will need programming tools to enable more effective use of available computational resources. Software for *visualization* and for large-scale scientific computation will be necessary to designers for an accurate view of material properties.

The ab-initio prediction of fundamental physicochemical and engineering properties of extended molecular systems is becoming feasible. This is being made possible by advances in atomic and electronic structure calculation, molecular dynamics simulation, and software and hardware design. Realistic predictions still rely heavily on adjustments to theory suggested by experimental verification.

Relevance

In the future, molecular modeling and simulation and high-throughput experimentation *will affect most products and processes* that depend on chemical, biological, and materials properties. This knowledge will generate new competitive advantages for modern industries, such as electronics and

optoelectronics, biotechnology, environmental technology, medical engineering, sensing and automation.

Computational modeling should provide a better understanding of the parameters and constraints for these nano-devices and create a framework for *interpreting experiments*. Modeling may even reduce the need for costly experimentation. Conceivably, modeling also could give new information about nanodevices that is not evident through experimentation alone.

Applications to be considered include drug design, high performance materials, catalysis, environmental processes, energy conversion, biotechnology, nanoelectronics, and nanomagnetics and the related field of nanotechnology. Affected industries include chemicals, pharmaceuticals and other biochemicals, paper, textile, electronics, and advanced materials.

Priorities

- Develop computational facilities and human resources to facilitate development of interdisciplinary centers and network to serve nanotechnology R&D activities. Collaboration among groups working in different disciplines and areas of relevance (chemistry, thermodynamics, mechanics, electronics, biological processes, others) will be encouraged.
- Multiscale and coupled phenomena modeling and simulation of nanostructures at the atomic and molecular level in order to further fundamental understanding, explore new phenomena, and improve design predictions, will be supported with priority.
- Develop new simulation and design software to systematically create new materials and systems for given properties and functions. Computational thrusts could focus on the modern advances of quantum chemistry, molecular mechanics, molecular dynamics and device modeling and prediction applied to the chemical, energy, environmental, and advanced materials technologies. The methods may include Quantum Mechanics (QM), Force Fields (FF), Molecular Dynamics (MD), Coarse Graining (CG), Statistical Mechanics (SM), and Continuum Parameters (CP). Simulations that incorporate multiscale/multiphenomena descriptions need to be developed.
- Development of software, computational approaches, and simulation tools for process control and molecular manufacturing. This area is a very timely topic as it focuses on the regime between atomistic simulations (quantum theory, molecular dynamics) and physicochemical engineering practice (process simulation and design). The idea here is to use the results of atomistic calculations to supplement experimental data in determining the parameters of the coarse grain, phenomenological models required for process simulation and design. The use of new data on structural correlations from the atomistic simulations should provide more detailed information not available from experiment and would lead too much more detailed and accurate predictions.

<u>Agency Participation and Partnerships</u>

NSF, DOD, DOE and NASA will develop a special focus on multiscale/multiphenomena simulation at the nanoscale. NSF and DOE will coordinate their respective announcements and the review process.

Example: NSF's "multi-scale, multi-phenomena theory, modeling and simulation at nanoscale" activity will provide funds for developing a national network where reference software could be found on the Internet. The emergence of new behaviors and processes in nanostructures, nanodevices and nanosystems creates an

urgent need for theory, modeling, large-scale computer simulation and design tools and infrastructure in order to understand, control and accelerate the development in new nanoscale regimes and systems. Research on theory, modeling and simulation of physical, chemical and biological systems at the nanoscale will include techniques such as quantum mechanics and quantum chemistry, multi-particle simulation, molecular simulation, grain and continuum-based models, stochastic methods, and nanomechanics.

User Facilities

Special Opportunities

The research scientists and engineers working in the area of nanotechnology will need access to state-of-the-art instrumentation and facilities for observation, characterization, manipulation and manufacturing. University-based and national laboratory-based centers will provide access to expensive equipment with rapid state-of-the-art changes.

The most common instruments will probably be various types of scanning probe, electron and ion microscopes. On the one hand, there has to be an understanding that a single research group can easily have need for several different scanning probe microscopes, since there are now many different types each optimized for a different task. On the other, the best electron and ion microscopes are very expensive and costly to maintain, and means should be provided for universities either to acquire, maintain and operate such systems, or have access to users facilities. There will also be a need for a wide range of facilities and instruments, ranging from synchrotron radiation and neutron sources, electron-beam and ion-beam manufacturing, all types of spectrometers and computational facilities to both handle the processing of massive amounts of data and carry out the crucial modeling/simulation work needed to advance the field rapidly. Since the emphasis for most of groups performing nanotechnology research needs to be on the science and not the equipment, the existing facilities (such as the National Nanofabrication Users Network) will be extended and a number of shared laboratories and regional facilities need to be funded and staffed.

The national laboratories have the capability to develop and maintain large–scale and multi–user neutron and photon facilities. Argonne National Laboratory is the site of the Advanced Photon Source and the Intense Pulsed Neutron Source; Oak Ridge National Laboratory houses the High Flux Isotope Reactor and will be the location of the Spallation Neutron Source; the Los Alamos Neutron Scattering Center, LANSCE, is located at the Los Alamos National Laboratory; the Lawrence Berkeley National Laboratory is the home of the Advanced Light Source; and the Stanford Synchrotron Radiation Laboratory is situated at the Stanford Linear Accelerator Center.

NIST has a Synchrotron Ultraviolet Radiation Facility and a Neutron Beam Split-core Reactor, high performance facilities to characterize nanostructures.

Priorities

- Multiple-user national centers and networks equipped with nanotechnology-specific equipment (type of measurement, industry, etc.) need to be funded and staffed; the centers may be based in universities or at national laboratories.

- Vertical integration of fundamental and technological research within the multiple-user centers will be encouraged for synergistic purposes. Multi-technology engineering demonstration facilities funded by mission-oriented agencies and industry should be included in the centers.
- Development and use of regional university-national laboratory-industry facilities will be encouraged.
- The issue of *information sharing* is paramount; an agency and specific funding might be identified to foster communication of ideas and results among the various subfields within nanotechnology. One approach would be for an agency such as NIST to sponsor a nanotechnology-specific information facility agreed by participating agencies.

<u>Agency Participation and Partnerships</u>

NSF's university-based user facilities and government laboratories will develop a system for key facilities in the U.S. All agencies will ensure that user facilities will be adequate for NNI.

Examples: The NSET Subcommittee will ensure there are no gaps in the development of the infrastructure and will avoid unnecessary duplication of effort. Each agency will retain responsibility for its own procurements. The working group will coordinate the activities related to management of hardware resources and management of the process of bringing cutting edge research to bear on development and deployment. The generic infrastructure will be developed through partnerships between sites that operate the hardware and the national research community. Center site selection will be determined as results of the peer review process. The agencies involved will issue parallel solicitations for proposals to establish these centers. The criteria for decision-making will be stated at the time of the solicitations.

NIH will support the infrastructure needed to accomplish the research goals of these projects, through (a) including in project budgets the funds needed to purchase equipment and services appropriate to the scale of the project, (b) funding of user fees at other nanotechnology facilities, and (3) infrastructure grants (e.g., through NCRR).

13. Societal Implications of Nanotechnology and Workforce Education and Training (total $28 million, $13 million above FY 2000)

<u>Vision and Strategy</u>

Vision

A university-based program is designed to provide effective education and training of nanotechnology professionals, especially for industrial careers. Focused research on social, economic, ethical, legal and workforce implications of nanotechnology will be undertaken.

The science, engineering, and technology of nanostructures will require and enable advances across a number of interrelated disciplines: physics, chemistry, biology, materials, mathematics, engineering and education. In their evolution as disciplines, they all find themselves simultaneously ready to address nanoscale phenomena and nanostructures. The dynamics of interdisciplinary nanostructure efforts will reinforce educational connections between disciplines and give birth to new fields that are only envisioned at this moment. Rapid development of nanotechnology will require changes in the laboratory and human resource infrastructure in universities, and in the education of nanotechnology professionals including lifelong learning.

A main objective of the national initiative is to provide new types of education and training that lead to a new generation of skilled workers in the multidisciplinary perspectives necessary for rapid progress in nanotechnology. The proposed initiative will leverage the existing strong foundation of nanoscience and engineering in the U.S., and will address the formidable challenges that remain.

When radically new technologies are developed, social, economical, ethical, legal, environmental and workforce development issues can rise. Those issues would require specific research activities and measures to take advantage of opportunities or reduce potential risks. NNI will address these issues in a program that will establish research into ethical, social, economic, and workforce impacts of information technology, including transformation of individuals and social institutions, impact of legislation and regulation, barriers to nanotechnology diffusion, and effective use of technology in education, ensuring that all Americans have the education to take advantage of high-wage jobs created in the new economy.

Special Educational Opportunities

Nanotechnology offers unprecedented opportunities to revitalize connection between disciplines and promote education at the interfaces between physics, mathematics, chemistry, biology and engineering. Although change is occurring in a relatively rapid fashion, there still exist many elements in the culture of our research universities that do not encourage multidisciplinary research. Specific suggestions to address these opportunities and needs are:

- *Introduce nanoscience and engineering in existing and new courses*. Courses on surface science, molecular dynamics, quantum effects, and manufacturing at molecular scale are necessary in curricula at the undergraduate and graduate levels. An integrative science and engineering approach is suggested. Technology programs cannot be developed without strong supporting science programs because of the scale and complexity of the nanosystems.
- Nanotechnology will help *integration of research and education into a new paradigm of learning based on molecular models* instead of microscopic approach. The recommended nanotechnology centers will provide an environment with facilities and interdisciplinary research teams that will enable educating a new generation of young scientists.
- *Educating and training a new generation of skilled workers* in the multidisciplinary perspectives necessary for rapid progress in nanotechnology is necessary. This represents a grand experiment in integration - integration of a multiplicity of disciplines and expertise, and integration of education and research into a true partnership. There should be a broader range of educational opportunities for students coming into nanotechnology areas. The students must become deep in one subject, but they also need to develop breadth by being able to transcend geographical location, institution and discipline. The problem with this goal is that most graduate students in technical areas are funded by the grants to their research advisors, and thus they are tied to a specific discipline and location because their mentors cannot afford to pay for students who are not in their labs. Thus, there should be a significant number of nanotechnology fellowships and training grants, which will give the best students the ability to craft their own education by specializing in one area but having the opportunity to work with one or more other mentors. This will further encourage a practice that is already occurring, since much of the current transdisciplinary nanotechnology research efforts are actually initiated by students who realize the benefits of working with more that one advisor. An emphasis on educational outreach is recommended for involving people at all levels.

- *Programs that encourage intermingling among science, engineering and business disciplines* should also be supported strongly, since grooming future technically competent entrepreneurs is at least as important as future professors and researchers. Nanotechnology workshops focused on graduate students should be held that allows them to see and understand the bigger picture, and encourage them to communicate across disciplinary boundaries.
- *Program to investigate societal impact of nanotechnology*, which will include focused research on social, economic, ethical, legal and workforce implications of nanotechnology.

Relevance
Education will need to address the fast development of nano-science and nano-industries. An entirely new generation will need to be trained in the sciences underpinning nanotechnology. The centers to be created in response to this initiative will strengthen the environment in which we train our young scientists and engineers, thereby helping to ensure that the United States will lead the technologically developed nations into the 21st Century. The creation of the intellectual capital is probably the most important long–term investment for science and technology.

The funding profile for university grants and national labs in nanotechnology must increase at a rate that will encourage the best young researchers to stay in the field and allow them to build up their own research programs. The first two products to come out of the early stages of government funding will be trained people and scientific knowledge. There must be a critical mass of these two before the development of a technology and intellectual property can occur. Once these become compelling, then actual products, the manufacturing infrastructure and the high paying jobs will arise that will repay the investments that have been made in this area.

Priorities and Modes of Support
To most effectively respond to the opportunities discussed above, several specific priorities are:
- Introduce nano-science and engineering in existing and new courses.
- Nanotechnology centers and networks, with facilities and interdisciplinary research teams, that will enable educating a new generation of young scientists.
- Create "regional coalitions" that involve industry-tech generation that include educational and training programs.
- Support student and post-doctoral fellowships for interdisciplinary work.
- Support student and young scientist internships at centers of excellence abroad.

Budget Request FY 2001: $28 million, a $13 million increase over FY 2000. Indirect contributions are from other funding themes, such as fundamental research and centers.

<u>Agency Participation and Partnerships</u>

NSF in collaboration with NIH, DOC and DOD and other agencies will establish an education and training program for the critical areas in nanoscience and engineering. An education and training network with the participation of all interested agencies is envisioned. University based centers will be co-funded by various agencies. DOC, DOD, DOE and NASA will offer opportunities for research work with university research centers to arrange for student and postdocs participation in research. NIH has in place several programs to support an additional prong of the NNI strategy, namely training and workplace issues that will be used for nanotechnology education and training.

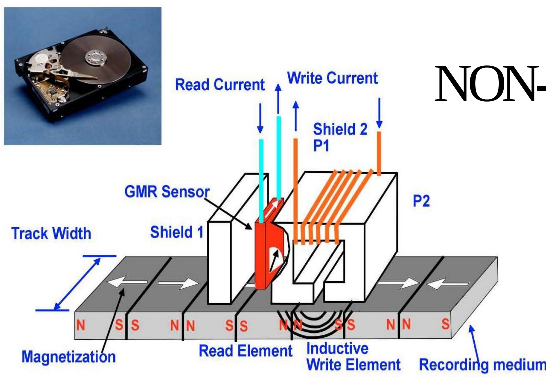
One specific example is the Mentored Quantitative Research Career Development Award program, initiated last year through the efforts of BECON and with cooperation from most of the NIH IC's.

Example: NSF's FY 2001 funding at $21 million ($12 million over FY 2000) will support student fellowships and traineeships, curriculum development on nanoscience and engineering, and for developing new teaching tools, as well as studies on the impact of nanotechnology on society from legal, ethical, social, economic and workforce perspectives. Exploitation of scientific and engineering advances at the nanoscale will bring along with it expected and sometimes unexpected impacts on society. The development and use of nanoscale technologies is likely to change the design, production and use of many goods and services, ranging from vaccines to computers to automobile tires. Studies might include (not exhaustive): economic assessments of the lifecycle of nanoscale development and use; business models for nanotechnology; how the public understands nanoscience and technology; the ethical and legal ramifications of nanotechnology in health, medicine, law, and the environment; knowledge barriers around the adoption of nanotechnology by commercial firms; an understanding of its diffusion patterns; and the implications of nanotechnology for everyday life.

APPENDIX A. Examples of nanotechnology applications and partnerships

(Additional examples are provided in the attached volume
"Nanotechnology Research Directions – IWGN Workshop Report", 1999)

GIANT MAGNETORESISTANCE IN MAGNETIC STORAGE APPLICATIONS



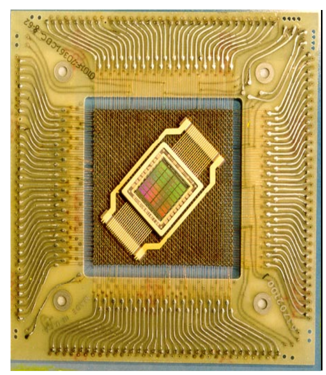
Magnetic recording process.

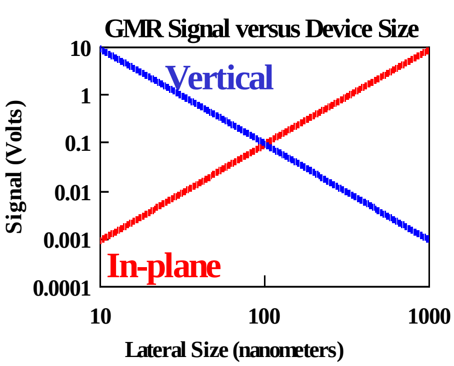
INFORMATION TECHNOLOGY

NON-VOLATILE HIGH DENSITY MEMORY

IN 1999: Within ten years from the fundamental discovery, the giant magnetoresistance (GMR) effect in nanostructured (one dimension) magnetic multilayers has demonstrated its utility in magnetic sensors for magnetic disk read heads, **the key component in a $34B/year hard disk market in 1998**. The new read head has extended magnetic disk information storage **from 1 to ~20Gbits**. Because of this technology, most of hard disk production is done by U.S.-based companies.

IN 3-5 YEARS: A future application of GMR is nonvolatile magnetic random access memory (MRAM) that will compete in the **$100B RAM market**. In-plane GMR promises 1Mbit memory chips in 1999; at the right, the size of this chip (center of image) is contrasted to an earlier 1Kbit ferrite core memory. Not only has the size per bit been dramatically reduced, but the memory access time has dropped **from milliseconds to 10 nanoseconds.** The in-plane approach will likely provide 10-100Mbit chips by 2002. Since the GMR effect resists radiation damage, these memories will be important to space and defense applications.



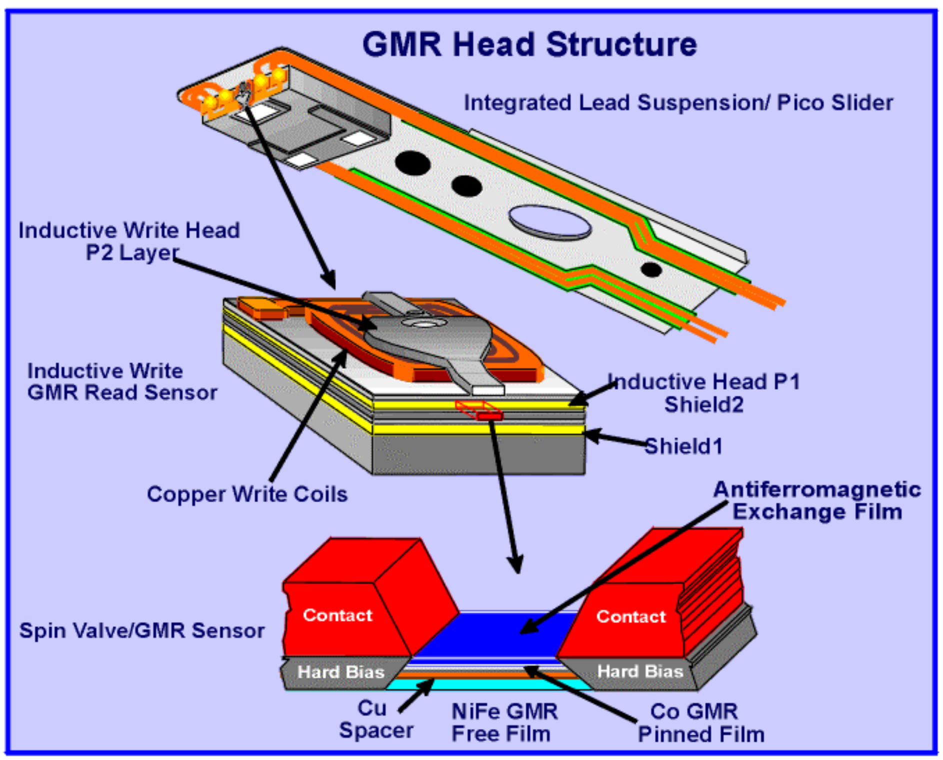


AFTER 5 YEARS: The in-plane GMR device performance (signal to noise) suffers as the device lateral dimensions get smaller than 1 micron. Government and industry are funding work on a vertical GMR device that gives larger signals as the device dimensions shrink. At 10 nanometer lateral size, these devices could provide signals in excess of 1 volt and memory densities of 10 Gbit on a chip, comparable to that stored on magnetic disks. If successful, this chip would eliminate the need for magneto-mechanical disk storage with its slow access time in msec, large size, weight and power requirements (**paradigm changes**)

Additional information:

A Commercial IBM Giant Magnetoresistance Read Head
Contact person: E. Grochowski, IBM

When certain kinds of materials systems are exposed to a magnetic field, their electrical resistance changes. This effect, called the magnetoresistive effect, is useful for sensing magnetic fields such as those in the magnetic bits of data stored on a computer hard drive. In 1988, the giant magnetoresistance effect was discovered in specially prepared layers of nanometer-thick magnetic and nonmagnetic films. By 1991, work at the IBM Almaden research center demonstrated that the GMR effect could be observed in easily made samples and that a special kind of GMR structure, a spin valve, could sense very small magnetic fields. This opened the door to the use of GMR in the read heads for magnetic disk drives. A commercial product based on this design was first announced by IBM in December 1997. In the spin valve GMR head shown in the figure below, the copper spacer layer is about 2 nm thick and the Co GMR pinned layer is about 2.5 nm thick. The thickness of these layers must be controlled with atomic precision.



Commercial IBM giant magnetoresistance read head.

NANOSTRUCTURED CATALYSTS

Researchers at Mobil Oil Co. have revolutionized hydrocarbon catalysis by the development of innovative nanostructured crystalline materials. Their program focused on zeolites, porous materials with well-defined shapes, surface chemistry and pore sizes smaller than 1 nanometer. A new zeolite class, ZSM-5 (see schematic in Figure 1) was discovered in the late 1960s. ZSM-5 has a 10 atom ring structure that contributes pore sizes in the range 0.45 – 0.6 nm (smaller than in zeolites X, Y and larger than in A) and enables shape selected chemistries not previously available.

Zeolite catalysts now are used to process over 7 billion barrels of petroleum and chemicals annually. New Zealand is using the same catalyst to produce 1/3 of its oil fuel requirement by converting it from natural gas via methanol and then high-octane fuels. ZSM-5, along with zeolite Y, now provide the basis for hydrocarbon cracking and reforming processes with a commercial value that exceeds $30B in 1999 (J. Wise, Vice President Exxon, ret.). Another example at Mobil Oil Co. is the aluminosilicate 10 nm shaped cylindrical pores (Figure 2), which has been applied in both catalysis and filtration of fine dispersants in the environment (Liu and Mou, 1996). Further systematic advances in nanotechnology are expected to increase its share of an overall world catalyst market that exceeds $210B in 1999.

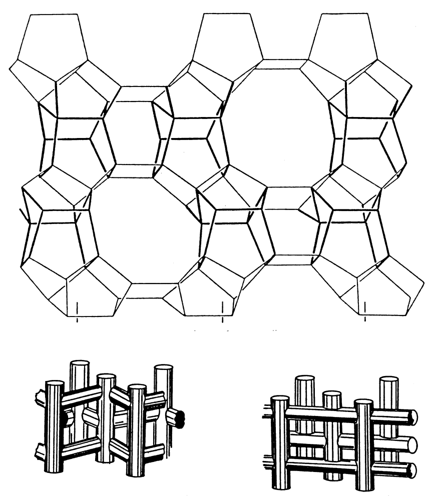


Figure 1. Schematic of the three dimensional channel structure of ZSM-5

Solid catalysts with one, two or three dimensions in the nanometer range can exhibit unique, tailorable activities. For instance, catalytic behavior of gold particles is turned on only after the particle diameter is smaller than 3-5 nm because those crystals have a special structure (icosahedral) that is different from bulk structure. A key objective of nanoscale catalyst research is increase of specificity, selectivity and yield in chemical reactors. Because of the improvements in nanostructured catalysts, desired product yields have increased significantly in the last decade.

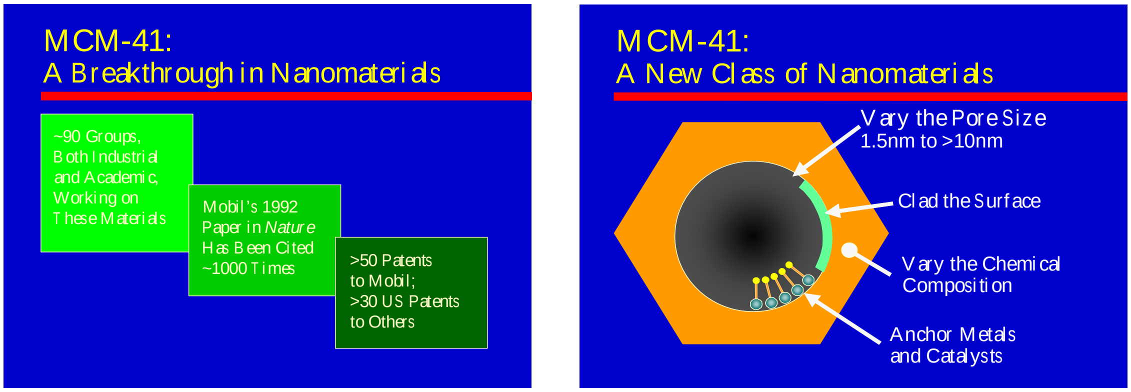


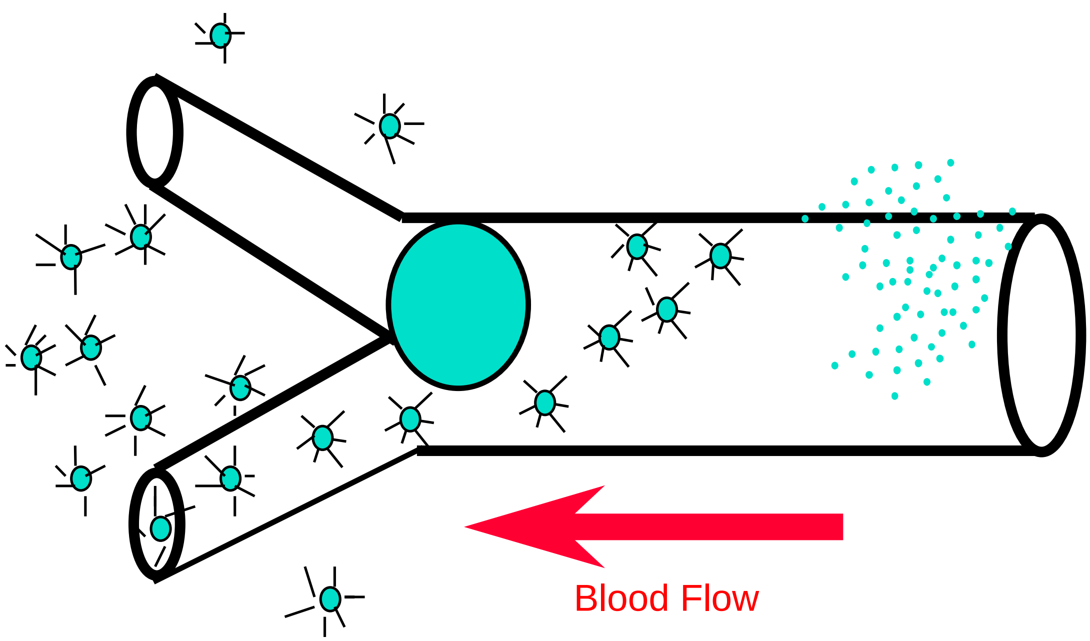
Figure 2. From discovery to application: a nanostructured material (MCM-41)

DRUG DELIVERY SYSTEMS

By using nanotechnology fundamental changes in drug production and delivery are expected to affect about half of the $380 billion worldwide drug production in the next decade. The U.S. company market share is about 40%. Nanotechnology will be used in various ways:

- Nanosizing will make possible the use of low solubility substances as drugs. This will approximately double the number of chemical substances available for pharmaceuticals (where particle size ranges from 100 to 200 nm).
- Dendrimer polymers have several properties (high solubility in aqueous solvent, defined structure, high monodispersity, low systemic toxicity) that make them attractive components of so-called nanobiological drug carrying devices.
- Targeting of tumors with nanoparticles in the range 50 to 100 nm. Larger particles cannot enter the tumor pores while nanoparticles can move easily into the tumor (Figure 1)
- Active targeting by adding ligands as target receptors on a nanoparticle surface. The receptors will recognize damaged tissue, attach to it and release a therapeutic drug.
- Increase the degree of localized drug retention by increasing the adhesion of finer particles on tissues
- Nanosized markers will allow for cancer detection in the incipient phase when only a few cancer cells are present.

An example of current commercialization is liposome encapsulated drugs produced by Nexstar (doxarubicin for cancer treatment and amphotericin B for fungal infection) with sales over $20 million in 1999.



In the 1980s, academic researchers proposed using polymers to embed nanoparticles carrying drugs (Douglas and Davis, 1987, "Nanoparticles in drug delivery"). This approach did not prove practical because of the difficulties in disposing of the polymeric blends after their use. In 1992, industry researchers proposed using nanocrystals without polymeric support (U.S. Patent 5,145,682, "Surface modified drug nanoparticles"). This solution has been adopted in the current applications.

<u>An example of industry-government partnerships</u> in this area is the project "Using nanosized particles for more effective cancer therapy" (NIST-ATP, NIH-NCI, CytImmune Sciences Inc., and EntreMed, Inc.). The partnership seeks to develop novel cancer therapeutics, using colloidal gold to effectively deliver biologics and gene therapies to targeted cells, thereby greatly improving the efficacy of the agents while reducing toxic side effects. Most drugs and other therapeutics have a systemic effect on healthy and unhealthy cells. There are often toxic side effects. The unique chemical properties of colloidal gold (tiny gold particles that remain evenly distributed in a solution) make it a promising vehicle for delivering drugs or genes to specifically targeted cells. Colloidal gold is already used as a protein marker by chemists and is also used for medical purposes. However, its therapeutic mechanisms are not completely understood. CytImmune Sciences, Inc. proposes to develop a novel cancer treatment using colloidal gold to deliver cytokines (which modulate the body's immune system) such as tumor necrosis factor. The company will evaluate the optimum size of the gold particles, study the pharmacokinetics and safety issues, and determine whether and how gold-cytokine complexes affect tumors. Studies evaluating colloidal gold for gene therapy to replace defective or missing genetic material also are envisaged. In the gene therapy research, the company will exploit the capability of a colloidal gold particle to bind and deliver genetic materials to target cells. CytImmune hopes to demonstrate cytokine treatment and gene therapy with enhanced safety and efficacy, enabling these cancer treatments to achieve their full potential. If successfully developed and commercialized, the technology could reduce the toxicity of many drugs and potentially enable therapies that harness the body's natural defenses. Colloidal gold is inexpensive to manufacture and therefore should be a cost-effective way of improving health. The ATP program will accelerate the collection of convincing preclinical data thus making it more probable that CytImmune can find a private-sector partner for conducting clinical trials. The research will be carried out in collaboration with the National Cancer Institute (Bethesda, Md.) and EntreMed, Inc. (Rockville, Md.). This 3-year project has received joint funding with $2 million from ATP/NIST and $1.7 million from industry.

NANOCOMPOSITES: NANOPARTICLE REINFORCED POLYMERS

Low-Cost, High-Strength Materials for Automotive Parts

Requirements for increased fuel economy in motor vehicles demand the use of new, lightweight materials - typically plastics - that can replace metal. The best of these plastics are expensive and have not been adopted widely by U.S. vehicle manufacturers. Nanocomposites, a new class of materials under study internationally, consist of traditional polymers reinforced by nanometer-scale particles dispersed throughout (Figure 1). These reinforced polymers may present an economical solution to metal replacement. In theory, the nanocomposite can be easily extruded or molded to near-final shape, provide stiffness and strength approaching that of metals, and reduce weight. Corrosion resistance, noise dampening, parts consolidation, and recyclability all would be improved. However, producing nanocomposites requires the development of methods for dispersing the particles throughout the plastic, as well as means to efficiently manufacture parts from such composites.

Dow Chemical Company and Magna International of America (in Troy, MI) have a joint Advanced Technology Program (ATP) sponsored by the National Institute of Science and Technology (NIST) to develop practical synthesis and manufacturing technologies to enable the use of new high-performance, low-weight “nanocomposite” materials in automobiles (NIST 1997). The weight reduction from proposed potential applications would save 15 billion liters of gasoline over the life of one year’s production of vehicles by the American automotive industry and thereby reduce carbon dioxide emissions by more than 5 billion kilograms. These materials are also likely to find use in non-automotive applications such as pipes and fittings for the building and construction industry; refrigerator liners; business, medical, and consumer equipment housings; recreational vehicles; and appliances.

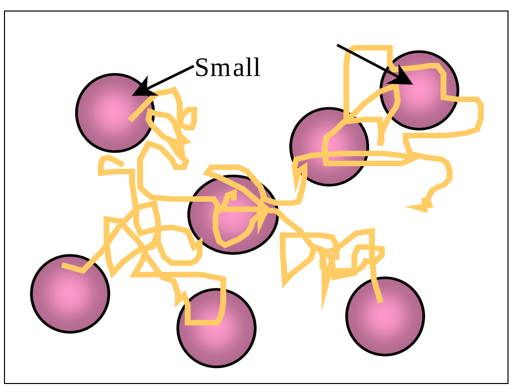
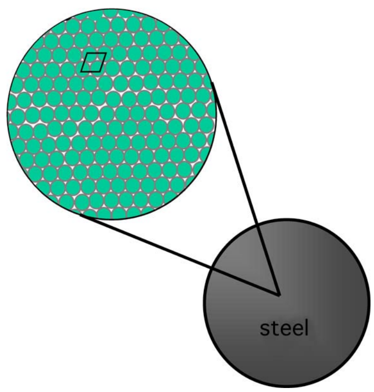


Figure 1. Schematic for nanoparticle-reinforced polymeric materials (after Schadler et al. 1998).

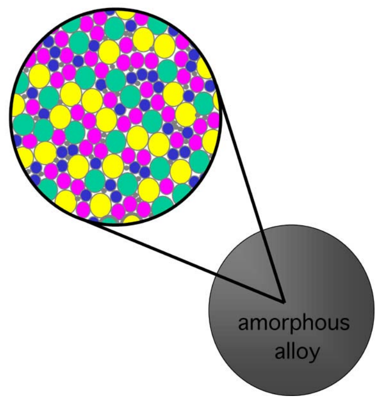
The ATP Ongoing Partnership has started in October 1997 for five years. The partnership includes: NIST-ATP, Dow Chemical Company, Magna International of America. Total project (est.) is $15.9 million with $7.8 million requested government funding.

AMORPHOUS METALS WITH CONTROLLED ATOMIC STRUCTURE

Increasing ability to design and fabricate materials atom by atom has allowed creation of new materials with customized physical and electronic properties. An example of such a material is the amorphous alloy called Vitreloy™ ($Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10.0}Be_{22.5}$) (1). The new material is twice as hard, twice as elastic, twice as strong and twice as tough as compared to steel. The rebounding and heat transfer properties are significantly different from the crystalline materials due to the different types of atoms and their arrangements (2).



The atoms in stainless steel are arranged in an ordered structure.



The 5 types of atoms which form the Vitreloy™ alloy are randomly arranged.

A crystalline solid, such as stainless steel, has a regular structure in which the atoms or molecules are arranged in a repeating pattern. The regular structure of crystalline solids is typically interrupted by defects. Examples of defects include impurities, missing atoms (a type of defect called a vacancy), and misaligned planes of atoms (another type of defect called a dislocation). Defects play an important role in determining the properties of a material. For example, even when the atoms in a solid are densely packed, the solid can be deformed due to the mobility of the defects and dislocations in the crystal. In contrast, an amorphous (noncrystalline) solid does not have a regular, periodic structure. The atoms in the amorphous alloy Vitreloy™ are in a densely packed, but random arrangement. Amorphous materials are formed by cooling the liquid material quickly enough to prevent crystallization; the atoms do not have time to arrange themselves into an ordered structure. Because of the varying sizes of these atoms and their random arrangement in the solid, there are no groups of atoms that can easily move past one another. A consequence of this low atomic mobility is the low internal friction when a force is applied.

Vitreloy™ [1], discovered at the California Institute of Technology by W.L. Johnson in 1993, can be cooled from the liquid state at rates as low as 1°C/s and still form a completely amorphous solid. This slow cooling rate is very unusual for amorphous metal systems that often need to be cooled at far faster rates in order to prevent crystalline phases from forming. The unique properties of amorphous solids make them useful in many commercial applications. One of the first applications of Vitreloy™ has been in the design of golf clubs. The amorphous alloy is two to three times stronger than many other conventional materials like titanium and steel. Other applications include projectiles to alter the structure of subterranean oil fields and different defense equipment.

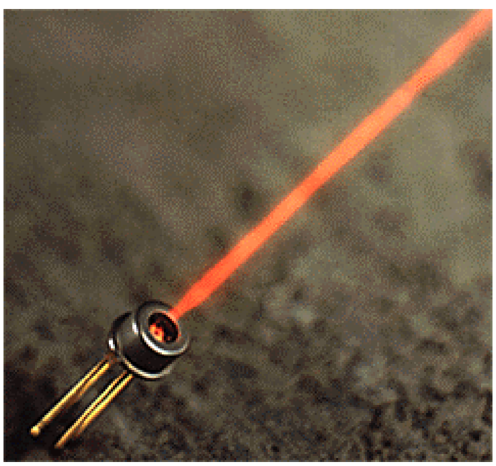
A demonstration can be made to highlight the interaction between a freely falling ball and the two metal plates, one of crystalline material and another of amorphous material. Some of the ball's kinetic energy will be converted to heat as it collides with either surface. Each collision causes movement of atoms in both the ball and the plate, and this motion is a kind of atomic friction that produces heat. In a perfectly elastic collision no kinetic energy would be lost, and the ball would bounce to its original height. The restitution coefficient is 0.71 for stainless steel and 0.99 for the amorphous alloy. Accordingly, one can measure twice the rebound on the first bounce of the steel ball on the amorphous alloy (98% versus 50%). The difference in the way the ball bounces on the two plates arises in large measure from the unusually low friction between the atoms of the amorphous metal as they move relative to one another during the ball-plate collision. This so-called "low internal friction" means that relatively little of the ball's kinetic energy is converted to heat, leading to a more trampoline-like bounce.

(1) Vitreloy ™ is produced by the Howmet Corporation.
(2) A. Peker and W.L. Johnson, *Appl. Phys. Lett*. **63**, 2342 (1993); W.L. Johnson, *Curr. Opin. Solid State Mat. Sci*. **1**, 383 (1996); W.L. Johnson, *Mater. Sci. Forum* **225-227**, 35 (1996).

TWO EXAMPLES OF NANOELECTRONIC DEVICES

The proposed National Nanotechnology Initiative would invest in the science base necessary to manufacture, characterize and utilize three dimensional nanostructured systems. While this goal is years away, technologies based on assemblies of one-dimensional nanostructures (superlattices) have already penetrated the marketplace. Two examples are High Electron Mobility Transistor (HEMT) and Vertical Cavity Selective Emitter Laser (VCSEL). These examples give an indication of the potential for nanoelectronics to completely change electronic devices in the next 10-20 years. Currently, other new concepts such as single electron devices, quantum cellular automata, and use of molecular and quantum devices are under investigation.

HEMT devices were engendered by the DoD 6.1 Ultra Small Electronics Research Program (USER, FY81-88) in which $60M was expended to develop technology capable of creating nanometer thick semiconductor films and electronic junctions. The DARPA Microwave Amplifier Front End Transistor (MAFET) program of FY92-99 used the HEMT devices as the major building block for sophisticated microwave and millimeter wave integrated circuits for radar and communications systems in various DoD applications. Today HEMT is used as a standard for the development of any military and commercial microwave or millimeter wave system requiring low noise figure and high gain. The commercial market for HEMT high frequency receiver/transmitter devices is estimated at $140M in 1997 with growth to $800M by 2002.

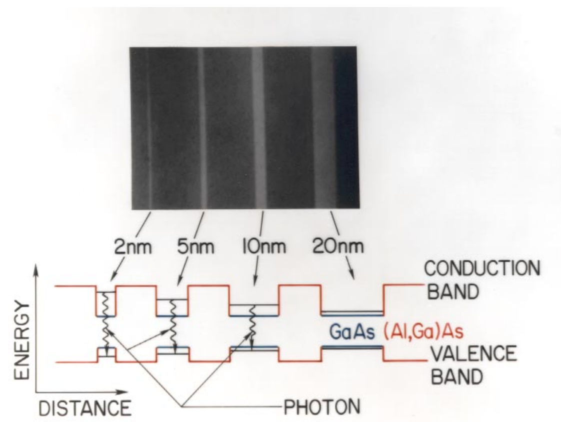


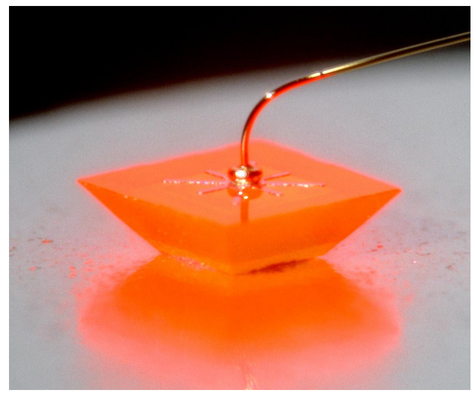
Vertical Cavity Surface Emitting Lasers are another device that relies on superlattices with nanometer thick films. VCSELs were first demonstrated in the 1970s by the Tokyo Institute of Technology (Japan) and became a commercial reality in the 1990s following innovations at ATT and DARPA funding. Fiberoptic data communications is the first major commercial application of VCELs, with a growing list of other applications such as optical sensors, encoder, range-finders, and extended range sensing. The present market is approximately $100M and is anticipated to grow to over $1B in the next 3-5 years. (A Honeywell VCSEL laser is shown in the picture and tabulated data below). The VCSEL has superior performance as compared to other solid state photon sources as shown in the following table:

	VCSEL	CD Laser	LED
Power Dissipation (mW)	20	100	200
Modulation Bandwidth (GHz)	>10	<2	>0.1
Wallplug Efficiency (%)	10	5	1

LED LIGHTING BREAKTHROUGHS FROM NANOTECHNOLOGY

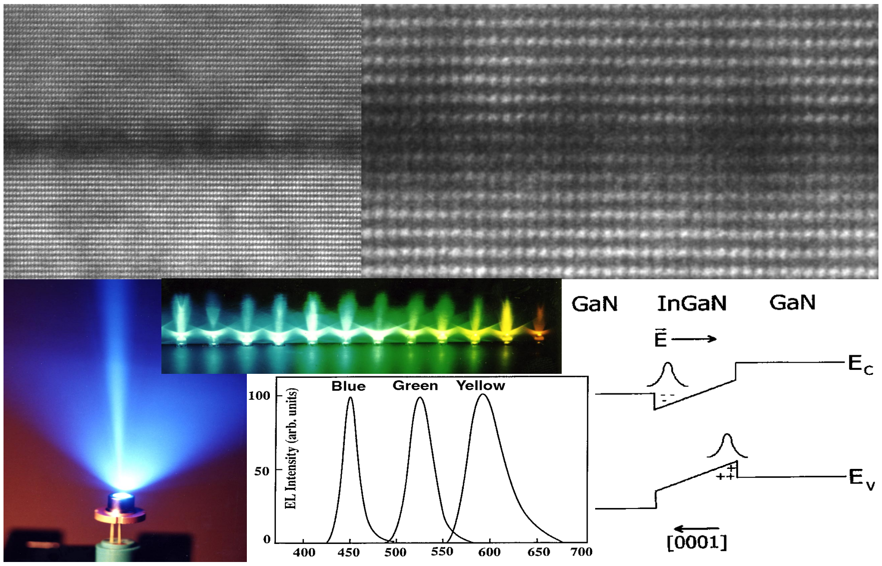
In the past decade, the ability to image and manipulate atoms has led to a revolution in lighting technologies (1-2). Historically, Edison's incandescent lamp, comprising a tungsten filament in a glass housing, has satisfied many of our lighting needs. When the filament is heated by passing electricity through it, some of the energy is emitted in the visible part of the spectrum and is accompanied by substantial generation of heat. In the United States, roughly 20% of all electricity is consumed for lighting, including both incandescent and fluorescent lights. This corresponded, in 1998, to a cost of $63 billion dollars. Moreover, there is a significant environmental impact from the approximately 112 million tons of carbon emission associated with providing this electricity.





Semiconductors used in the preparation of light emitting diodes (LEDs) for lighting can increasingly be sculpted on nanoscale dimensions, as presented in the first schematic (by Tom Kuech, U. of Wisconsin). Electrons in such semiconductors can be physically trapped in nanoscale "boxes" that are constructed out of different materials with atomic scale precision. When electrons in these boxes are excited electrically as part of LEDs, they emit particular colors of light that are controlled by the size of the box in which they are trapped, the number of such boxes, and the particular combination of atoms used in the construction of the boxes. A chip-shaped super-efficient (45%) red LED with embedded nanoscale heterostructures is shown in the second picture (3). An illustration of nanoscale architecture used to tune the color of light emitted by an LED is represented in the third picture.

The images are taken by high-resolution transmission electron microscopy. The horizontal planes are the (0001) planes in the wurtzite structure, about 0.51 nm. Thus, the width of the quantum well is 1.5 nm or three basal plane spacing. The horizontal separation corresponds to 0.276nm, the (1-100) spacing, which is close to the interatomic separation in GaN.



White lighting would represent an enormous market for LEDs in households and workplaces. Several methods can be used to produce white LED lighting, including combinations of colored LEDs and use of a single blue LED in combination with a phosphor. These "white LEDs" will require a substantial investment in nanotechnology through development of advanced, efficient LEDs and phosphors. The ability to exert atomic scale control over the placement of atoms suggests that yet greater efficiencies can be realized through customized creation of nanoarchitectures like semiconductor dots, huts, and films. Since the discovery that semiconductor structures could be coaxed into emitting light by modest battery-scale voltages, there has been a phenomenal increase in the efficiency with which these light emitting diodes (LEDs) operate. These tiny devices, typically a fraction of a millimeter on a side, reflect our ability to deposit atoms that lead to semiconductors virtually an atomic layer at a time. The efficiencies of LEDs now rival incandescent light sources in many parts of the visible spectrum and are finding applications in displays, automobile lights, traffic lights and indicators, because of their compactness, durability, and low heat generation. A spectacular example is the NASDAQ sign at Times Square in New York that boasts nearly 19 million LEDs!

Projections indicate that such nanotechnology-based lighting advances have the potential to reduce worldwide consumption of energy by more than 10%, reflecting a savings of $100 billion dollars per year and a corresponding reduction of 200 million tons of carbon emissions. Furthermore, an estimated 125 gigawatts of electricity generating capacity could be reallocated or need not be created, which could save over $50 billion dollars in construction costs.

1. High Brightness Light Emitting Diodes; G.B. Stringfellow and M. George Craford, Volume Editors, Academic Press, San Diego, 1997.
2. F.A. Ponce, D. P. Bour, "Nitride-based semiconductors for blue and green light-emitting diodes", Nature, 1997, 386, 351-359.
3. "The Case for a National Research Program on Semiconductor Lighting", R Haitz, F. Kish, J. Tsao, J. Nelson, 1999 Optoelectronics Industry Development Association forum, Washington D.C., October 6, 1999.

NATIONAL SECURITY: BIO DETECTION

Nanotechnology promises revolutionary advances in military capability. The confluence of biology, chemistry, and physics at the nanometer scale is enabling significant advances in sensors for biological and chemical warfare agents. Civilian disaster response teams and medicine will benefit as well. We cannot afford to respond to a nerve gas attack, such as the 1995 Aum Shinrikyo incident in Japan, by carrying a canary as a sensor. Defense research and development programs are pursuing many sensor options; two related technologies are nearing fruition.

One is a colorimetric sensor (Figure 1) that can selectively detect biological agent DNA; it is in commercial development with successful tests against anthrax (and tuberculosis) (C. Mirkin, Northwestern University). DNA is attached to nanometer size gold particles; when complementary DNA strands are in solution, the gold particles are bound close to each other. The nanoparticles change the suspension color as a function of the particle clustering. . Compared to present technology, the sensor is simpler, less expensive (by about a factor of 10), and more selective.

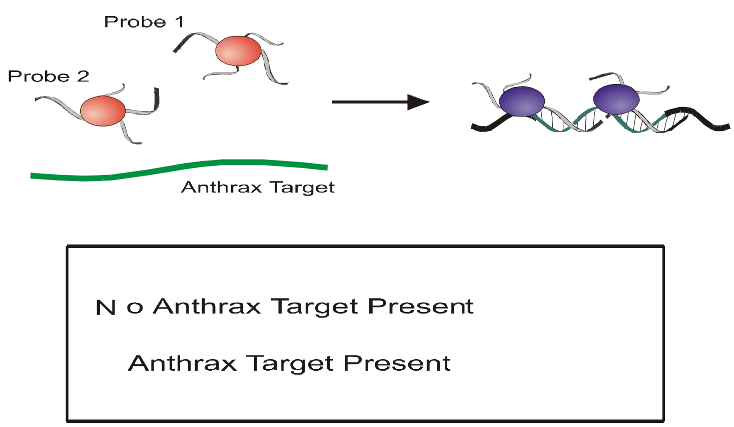


Figure 1. Anthrax detection: when the anthrax target is present, pairs of nanoparticles assemble together via the DNA filaments and change the color of the suspension.

A complementary effort is based on atomic force microscopy (AFM) in which a sandwich immunoassay attaches magnetic beads to a microfabricated cantilever (R. Colton, NRL). In the laboratory the AFM technology is already 100 to 1,000 times more sensitive than conventional immunoassays.

Both colorimetric and magnetic bead technologies might be implemented in detector arrays that provide simultaneous identification of multiple pathogens.

1. “Colorimetric DNA-Detection,” R. Elghanian, J.J. Storhoff, R.C. Mucic, R.L. Letsinger, and C.A. Mirkin, Science 277, 1078 (1997); “One-pot Colorimetric DNA Differentiation of Polynucleotides with Single Base Imperfections Using Au Nanoparticle Probes,” J.J. Storhoff, R. Elghanian, R.C. Mucic, C.A. Mirkin and R.L. Letsinger, J. Am. Chem. Soc. 120, 1959 (1998).
2. “Sensing Molecular Recognition Events with Atomic Force Microscopy,” G.U. Lee, D.A. Kidwell and R.J. Colton, Langmuir 10, 354 (1994); “A High Sensitivity Micromachined Biosensor,” D.R. Baselt, G.U. Lee, K.M. Hansen, L.A. Chrisey and R.J. Colton, Proc IEEE 85, 672 (1997).

WATER PURIFICATION AND DESALINIZATION

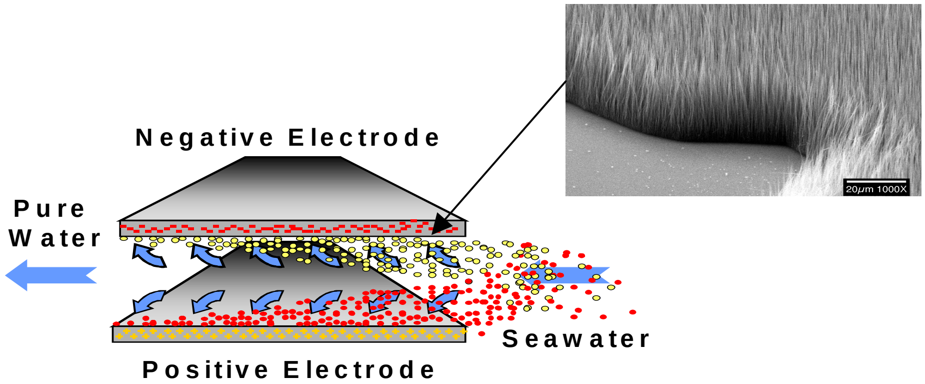
An energy-efficient Flow Through Capacitor (FTC) technology for water desalinization has been designed to desalt seawater with at least 10 times less energy that state-of–the art reverse osmosis and at least 100 times less energy than distillation. The energy usage of the FTC is anticipated to be less than 0.5 Whr/liter and is being designed for portable use as well as for large-scale integration. The capital cost and operational costs over a 5 year period are predicted to be approximately a factor of 3 less than reverse osmosis systems. The critical experiments underpinning these estimations are underway now. This energy-efficient process is possible by fabricating of very high surface area electrodes that are electrically conductive using aligned carbon nanotubes, and by other innovations in the system design.

The DARPA-funded flow through capacitor desalinization technology being developed by Marc Andelman, its inventor at Biosource Inc, and collaborators at Sabrex of Texas, Nanopore Inc. and Boston College, is a common sense approach based on several technological advances which takes the salt out of seawater as opposed to reverse osmosis with takes the water out of the salt.

The FTC is configured as a deionizing water filter using very high surface area capacitor electrodes (1000 m^2/g). Upon supplying a small dc voltage (1-2 V), the seawater is rapidly purified due to the fact that the dissolved ions become electrostatically attracted to the high surface area electrode materials. The positively charged ions (Na^+, Ca^{++}) are attracted to the negatively charged electrode, while the negatively charged ions (Cl^-, $SO3^-$) in the water are electrostatically attracted to the positively charged electrode as shown in the figure below. The performance of the FTC is rooted in nanotechnology, which enable the fabrication of novel high surface area conductive electrode materials to reduce resistive losses and increase charged ion (Na, Cl, etc.) adsorption capacity. The highly conductive materials will reduce resistive losses of the electrodes and makes the desalting process energy-efficient.

Global population is increasing while fresh water supplies are decreasing. The UN predicts that by the year 2025 that 48 countries will be short of fresh water accounting for 32% of the world's population! Water purification and desalinization are some of the focus areas of preventative defense and environmental security since they can meet future water demands globally. Consumptive water use has been increasing twice as fast as the population and the resulting shortages have been worsened by contamination.

Marc Andelman, U.S. Patents: US 5,192,432, 5,196,115, 5,200,068, 5,360,540, 5,384,685, 5,415,768, 5,425,858, 5,620,598



High surface area, high-conductivity electrodes from aligned carbon nanotubes
(after Biosource Inc., Sabres of Texas and Boston College)

NANOPHASE TECHNOLOGIES CORPORATION:
A SMALL BUSINESS FOCUSED ON NANOTECHNOLOGY

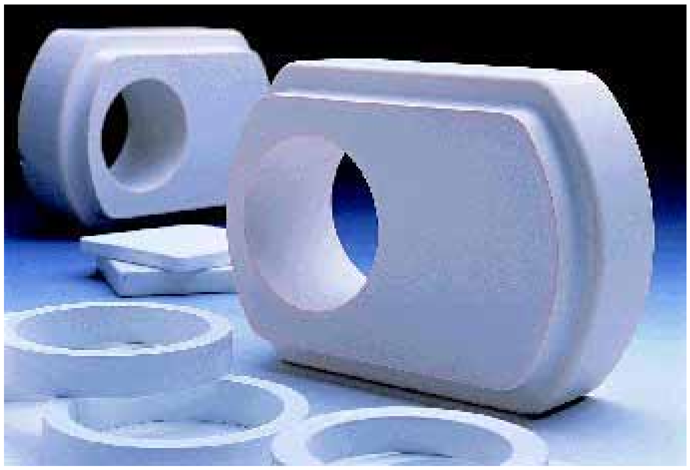
In 1985, the Office of Basic Energy Sciences, DOE began supporting a research activity in the emerging field of nanophase materials at Argonne National Laboratories' Materials Science Division. Nanophase materials involve powders made of extremely small crystals, which are compacted to yield solid materials. Because the grain sizes are so tiny, one can obtain enhanced plasticity, chemical reactivity, optical absorption, magnetism or other properties.

Initially, the materials were too poorly understood to be developed for industrial applications, but by 1989, Argonne Researcher Dick Siegel (now at Renssellaer Polytechnic Institute) felt confident enough to start a small company commercializing nanophase products. Nanophase Technologies (NTC). Initial funding for NTC was supplied by ARCH, through their associated venture capital fund, and by the State of Illinois, through grants for new job creation. Subsequent funding was raised from a consortium of venture capital funds, and from private individuals and groups. An additional source of funding that was very important to NTC's development was an ATP grant from the Department of Commerce (in 1992), which enabled the company to develop its patented physical vapor synthesis (PVS) process for manufacturing nanocrystalline materials in commercial quantities. This process was based on the laboratory-scale technology used at ANL from 1985 onward. NTC has also developed complementary nanoparticle coating and dispersion technologies, including its proprietary discrete particle encapsulation (DPE) process, as well as capabilities for superplastic forming of ceramic parts. Together, these technologies have enabled NTC over the past decade to enter a number of viable commercial markets. The company presently employs about 40 full-time workers (about 15 of whom hold advanced degrees) in its suburban Chicago facility. NTC currently targets several markets: electronics (including advanced electronics, electromagnetic radiation protection, and advanced abrasives for chemical mechanical polishing); ceramic parts; specialty coatings and catalysts; and other technologically similar applications. In each of these market areas, NTC establishes collaborative relations with major corporate customers to develop and jointly implement nanoscale solutions for the customer's needs. In many cases, products developed to satisfy a particular market need also have significant applicability across other markets. For instance, materials used in conductive coatings also have applicability for antistatic coatings and conductive strip carriers for color toners, abrasives, cosmetics and near-net shaping of ceramic parts. The NTC Web site provides current updates: http://www.nanophase.com.

Additional information on the government-industry partnership funded by ATP/NIST:

"Synthesis and Processing of Nanocrystalline Ceramics on a Commercial Scale" (1992)

- ATP funding enables a 25,000-fold increase in production of materials made of nanosized particles and a 20,000-fold reduction in cost per gram (from 10 grams of material per day at $1,000 per gram to the current capacity of 100 tons per year at 5 cents per gram).
- Sunscreens made with these materials are on the market, offering increased protection levels.
- Tests of prototype products made with these materials show that mechanical seals gain up to 10-fold increases in service life and industrial catalysts become up to four times more active.



Materials made of nanoparticles finally achieve their promise through a government-industry partnership

The ATP funding also was used to refine and demonstrate a process for shaping nanoscale ceramics into parts quickly and economically, without machining. The company president credits the ATP with helping Nanophase attract major industry collaborators and millions of dollars in venture capital funding, leading to an agreement to distribute the materials in more than 300 countries. The materials are used in a number of commercial products, including cosmetics and skin-care sprays and powders. Independent tests show that sunscreens containing nanocrystalline titania (a non-irritating alternative to sun-blocking chemicals) provide higher SPF protection using less material by weight than do conventional products, with no skin-whitening effect. Nanophase began making commercial quantities of material in late 1996 and reported $2.24 million in sales for the first nine months of 1997. Applications include semiconductor polishing slurries, ceramic armor, parts for medical devices, and industrial catalysts. ATP funding was $944K, and non-ATP funding was $2 million.

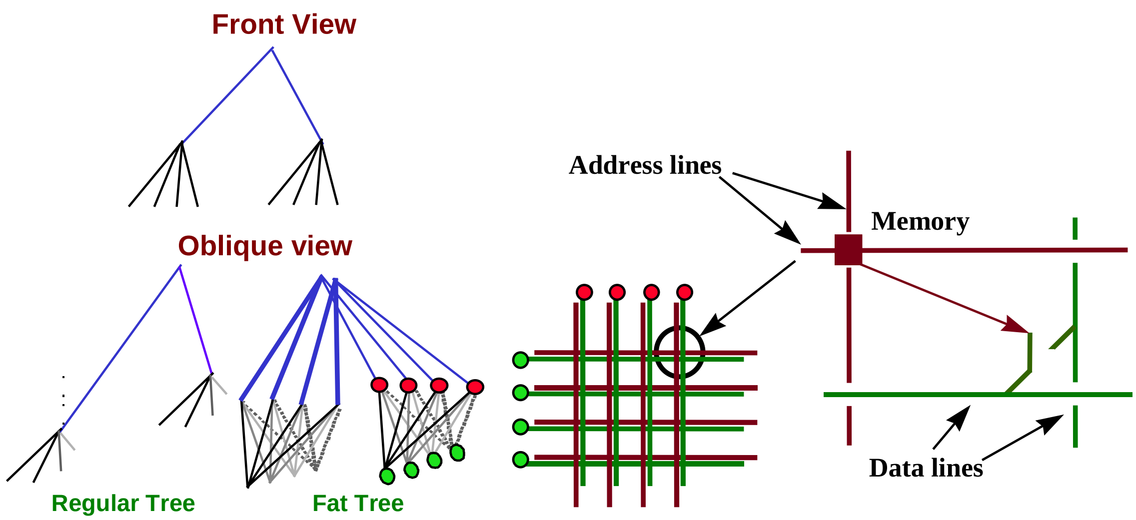
MOLECULAR ELECTRONICS
UCLA-HP project sponsored by NSF and DARPA

J. Heath (UCLA) and S. Williams (Hewlett-Packard Laboratories), in a NSF GOALI supported activity (Awards 94-57712 and 95-21392) have taken steps towards a new way to circumvent problems that will arise in the semiconductor industry when circuit feature sizes reach below the resolution of optical lithography.

If the reduction in size of electronic devices continues at its present exponential pace, the size of entire devices will approach that of molecules within two decades. However, well before this happens, both electronic devices and the manufacturing procedures used to produce them will have to change dramatically. This is because current devices are based primarily on classical mechanics, but at the scale of molecules, electrons behave as quantum mechanical objects. Also, the cost of factories for fabricating electronic devices is increasing at a rate that is much larger than the market for electronics; therefore, much less expensive manufacturing process will need to be invented.

Thus, an extremely important area of research is *molecular electronics*, in which molecules with electronics functionality are designed. synthesized using the batch processes of chemistry, and then assembled into useful circuits through the processes of self-organization and self-alignment. A major limitation of any such process is that chemically fabricated and assembled systems will necessarily contain defective components and connections. This limitation was addressed in a 1998 paper entitled “A Defect-Tolerant Computer Architecture: Opportunities for Nanotechnology” in *Science* 280:1716-1721. By describing a silicon-based computer that was designed to operate perfectly in the presence of huge numbers of manufacturing defects, researchers from Hewlett-Packard Labs and UCLA presented an architectural solution to the problem of defects in molecular electronics, as described in Figure 1, and thus demonstrated in principle that manufacture by chemical assembly is feasible.

In 1999, researchers from HP Labs and UCLA experimentally demonstrated the most crucial aspect for such a system, an electronically addressable molecular switch that operates in a totally “dry” environment (Collier et al. 1999). Logic gates were fabricated from an array of configurable molecular switches, each consisting of a monolayer of electrochemically active rotaxane molecules, as illustrated in Figure 2, sandwiched between metal electrodes.



a) Tree Architectures b) The Crossbar

Figure 1. The logical design of a defect-tolerant circuit: (a) shows a “fat tree” architecture in which every member of a logical level of the tree hierarchy can communicate with every member at the next level. In the case of a defective component, these structures enables one to route around and avoid the defect; (b) shows how this architecture is implemented using cross bars, which are very regular structures and look like something that can be built chemically. The complexity required for a computer is programmed into the crossbars by setting the switches to connect certain elements of the tree together. Using silicon circuitry, two completely separate sets of wires (address and data lines) are required for the cross bars and seven transistors are required for each switch, since a continual application of electrical power is required to hold the sense of the switches.

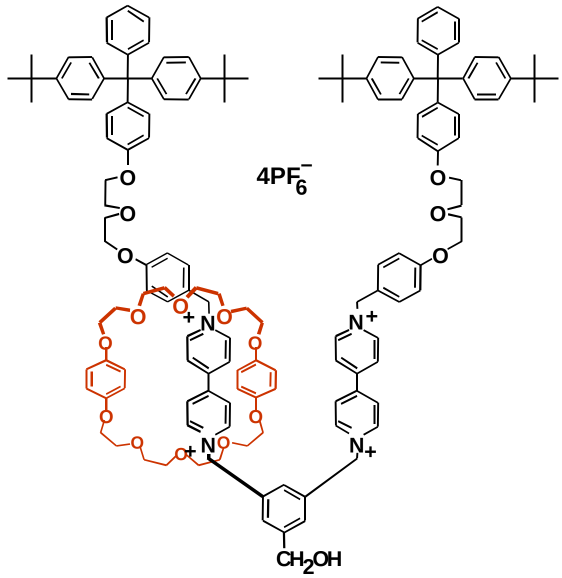


Figure 2. The atomic structure of the rotaxane molecule used in the devices described above as a molecular switch. This molecule conducts electrons via resonant tunneling through unoccupied molecular orbitals when it is in its reduced chemical state (switch closed), but it is a tunneling barrier in its oxidized state (switch open). The switch can be closed electronically in a solid-state circuit by applying the appropriate voltage across the molecule.

EDUCATION ACTIVITIES IN NANOSCALE SCIENCE AND ENGINEERING (EXAMPLES)

A. Courses on Nanoscale Science and Engineering Offered in U.S. Universities

Advanced quantum devices, University of Notre Dame (EE 666)
Nano-course, Cornell Nanofabrication Facility (A. Clark, M. Isaacson)
New technologies, University of Wisconsin, Madison (R. Hamers)
Nanostructured materials, Renssellaer Polytechnic Institute (R. Siegel)
Colloid chemical approach to construction of nanoparticles and nanostructured materials, Clarkson University (J.N. Fendler)
Nanoparticles processes, Yale University (D. Rosner)
Nanorobotics, South California University (A. Requicha)
Nanotechnology, Virginia Commonwealth University (M. El-Shall)
Chemistry and physics of nanomaterials, University of Washington (Y. Xia)
Scanning probes and nanostructure characterization, Clemson University (D. Correll)
Nano-scale physics, Clemson University (D. Correll)
“Capstone” course on nanotechnology “hands-on” for two-year colleges at the Penn State University Fabrication Facility (S.J. Fonash)

B. Education and outreach information on nanoscience and engineering through Internet (http://mrsec.wisc.edu/edetc)

The objective of this website is to introduce viewers to the tools that let us "see" atoms, manipulate them, and create nano-architectural wonders. Viewers can investigate the frontiers of the nanoworld by learning how materials are customized to create everything from atomic trampolines to DNA to ferrofluids to semiconductors that give off blue light!

This site is a resource for education and outreach efforts associated with the National Science Foundation-supported Materials Research Science and Engineering Center on Nanostructured Materials and Interfaces based at the University of Wisconsin-Madison.
Wisconsin outreach (MRSEC, contact Prof. A. Ellis, ellis@chem.wisc.edu)

Another website for education and outreach in nanoscale science and engineering has been established by University of North Carolina (www.cs.unc.edu/research/nano).

C. Education and Training for Nanophases in the Environment, Agriculture and Technology

NEAT (Nanophases in the Environment, Agriculture and Technology) is a multidisciplinary research and education program which links the fundamental physics, chemistry, and engineering of small particles and nanomaterials to several challenging areas of investigation:

- Applications in ceramic, chemical, electronic, environmental, and agricultural technology
- Environmental transport and transformation and resulting roles in environmental pollution and remediation
- Interactions with the biosphere, especially microorganisms
- Effects on health.

NEAT (http://neat.ucdavis.edu) has been established through the IGERT (Integrative Graduate Education, Research and Training) Program funded by NSF at the University of California Davis. Program contact is Prof. Alexandra Navrotsky, Department of Chemical Engineering and Materials Science (anavrotsky@ucdavis.edu).

The NEA-IGERT program involves 14 faculty in eight departments in four colleges : the College of Engineering, the Collage of Letters and Science, the College of Agricultural and Environmental Sciences, and the College of Veterinary Medicine. .The program offers funds for the support of 14 Ph.D. students per year. Students in four year doctoral programs will generally receive about half their funding from the IGERT. Over the course of its five years, NEAT will have 50-60 graduate student and 10-20 undergraduate student participants. By bringing together faculty and students in fields ranging from the nanotechnology of electronic materials to the interaction of nanoparticles in soils, water, and air with living organisms, this program will both educate students broadly and provide a basis for exploring common features of nanomaterials originating in many different ways. Such a broad understanding may help answer, in the long term, questions about the stability of devices based on nanotechnology (including what happens when obsolete devices are discarded), and may help in the design, synthesis, and application of new classes of nanomaterials and technology delivered from them.

D. K-12 education on Nanofabrication Manufacturing Technology at Penn State (Nanofabrication Facility, 185 Materials Research Institute Building, The Pennsylvania State University, University Park, Pa. 16802)

The Nanofabrication Manufacturing Technology (NMT) Program is a Commonwealth funded initiative based on sharing the Penn State Nanofabrication Facility (including the NSF-sponsored National Nanofabrication Users Network) among Pennsylvania institutions. Using the resource-sharing approach, the program addresses the tasks of (1) enhancing workforce development, (2) improving K-12 science and technology education, (3) increasing educators' awareness of Nanofabrication-based technologies, and (4) providing research and development assistance to Pennsylvania industry. The NMT Program has the goals of increasing job opportunities for Pennsylvanians and of nurturing and growing nanofabrication, semiconductor, and semiconductor-supplier industries in the Commonwealth.

ACADEME-INDUSTRY-GOVERNMENT PARTNERSHIPS

Federal and local governments (N.Y., N.J., Minnesota, Kentucky, Washington, NC, others), private profit (industry) and non-profit organizations (such as Beckman Institutes), and academic institutions have all determined that nanoscale science and engineering is an important long-term field for investment.

Examples of universities with investments in nanotechnology in the last few years are:

- Arizona State University: Nanostructure Research Group
- California Institute of Technology: Materials and Process Simulation Center [http://www.theory.caltech.edu/~quic/index.html]
- Cornell University: Cornell Nanofabrication Facility [http://www.nnf.cornell.edu]; Cornell Science and Technology Center (NSF) in Nanobiotechnology
- Georgia Institute of Technology: Nanocrystal Research Laboratory; Nanostructure Optoelectronics
- Johns Hopkins University: Center for Nanostructured Materials http://www.pha.jhu.edu/groups/mrsec/main.html
- Massachusetts Institute of Technology: NanoStructures Laboratory [http://www-mtl.mit.edu/MTL/NSL.html]
- Materials Research Science and Engineering Centers (MRSECs) with interdisciplinary research groups addressing nanostructured materials. For links to their web sites see http://www.nsf.gov/mps/dmr/mrsec.htm
- National User Facilities (NSF sponsored) in x-ray synchrotron radiation, neutron scattering, and high magnetic fields provide access to major facilities for the benefit of researchers in a wide range of science and engineering fields including nanoscience and engineering. See http://www.nsf.gov/mps/dmr/natfacil.htm
- NNUN is a partnership involving NSF and five universities (Cornell University, Stanford University, UC Santa Barbara, Penn State University and Howard University). See http://www.nnun.org/
- Northwestern University (IL): Center for Nanofabrication and Molecular Self-assembly. See http://www.chem.nwu.edu/NanoWeb/index.html
- Oxford Nanotechnology (MA): Molecular nanotechnology, nanolithography
- New Jersey Institute of Technology: Nonlinear Nanostructures Laboratory (NNL)
- Pennsylvania State University: Nanotechnology
- Princeton University: Nanostructure Laboratory
- Rice University: Center for Nanoscale Science and Technology (fullerenes)
- Stanford University: Stanford National Nanofabrication Users Network (NNUN) [http://snf.stanford.edu/NNUN]; [http://feynman.stanford.edu/qcomp]
- University of California, Santa Barbara: NSF Science and Technology Center for Quantized Electronic Structures (QUEST)
- University of Florida, The Center for Research at the Bio/Nano Interface, Department of Chemistry

- University of Illinois at Urbana-Champaign: Beckman Institute [http://www.beckman.uiuc.edu/themes/MENS.html]; STM Nanofabrication and Characterization Group
- University of Notre Dame: Center for Nanoscience and Technology
- University of Texas at Arlington: NanoFAB Laboratory [http://engineering.uta.edu]
- University of Washington: Center for Nanotechnology
- University of Wisconsin, Madison: Center for Nanostructured Materials and Interfaces http://mrsec.wisc.edu/
- Washington State University: Nanotechnology Think Tank
- Yale University: Optoelectronic Structures/Nanotechnology

Examples of Federal and industry research programs collaborating with academe:

- California Molecular Electronics Corporation (CALMEC): Molecular Electronics
- Defense Advanced Research Projects Agency (DARPA): The ULTRA Program [http://web-ext2.darpa.mil/eto/ULTRA/index.html]
- Hewlett Packard Lab: TERAMAK program
- IBM: Nanotech program [http://www.almaden.ibm.com/vis/vis_lab.html]
- IBM's Zurich Research Laboratory: Microscopy at the atomic level
- MITRE Corporation: Covers topics on nanoelectronics and nanocomputing [http://www.mitre.org/technology/nanotech]
- Molecular Manufacturing Enterprises, Inc.(MMEI)
- Molecular Nanotechnology NanoLogic, Inc.: Integration of nanotechnology into computers
- Nanogen Co.: nanomanufacturing on a chip
- Nanophase Technologies Corporation
- NanoPowders Industries
- NanoSystems Co.: Drug delivery
- Nanotechnology Development Corporation
- NASA: Nanotechnology, Nanoelectronics [http://www.nas.nasa.gov]
- National Institute of Standards and Technology (NIST): Nanostructure fabrication
- Naval Research Laboratory (NRL): Nanoelectronics processing facility and Surface Nanoscience {http://stm2.nrl.navy.mil]
- National Science Foundation (NSF): Partnership in Nanotechnology [http://www.nsf.gov/home/crssprgm/nano/start/htm]; Nanoscale processes in biological systems [http://www.nsf.gov/nano]
- Office of Naval Research (ONR): Nanotechnology, nanoelectronics
- Raytheon Co.: nanoelectronics
- Texas Instruments: projects on QMOS program and TSRAM: Tunneling-based static RAM
- Xerox Palo Alto Research Center (PARC): Nanotechnology, molecular nanotechnology [http://nano.xerox.com/nano]
- Zyvex: Molecular manufacturing.

Illustrations of partnerships:

Government - Industry Partnerships

Three example partnerships supported by ATP/NIST spanning about seven years in advanced materials relying on unique properties of nanosized particles. These examples show the breadth of application (medical to cosmetics to automotive) and industrial interest (small business to large corporation) and rough time scale for commercialization (less than 10 years). These examples are purposely shown in the one narrow nanotechnology R&D field of nanoparticles. The examples further show that government-industry partnerships can play a key role in aiding U.S. industry speed nanotechnology innovations into the marketplace.

- Just started partnership – Nanoparticles for cancer therapy: NIST-ATP, NIH-NCI, CytImmune Sciences Inc., and EntreMed, Inc., “Using nanosized particles for more effective cancer therapy”
- Ongoing partnership – Nanocomposites for the automotive industry: Industry-Government Partnership: NIST-ATP, Dow Chemical Company, Magna International of America “Nanocomposites: Materials for Automotive Parts”
- Past Partnership, now fully commercialized – Nanoparticle synthesis: NIST-ATP and Nanophase Technologies “Synthesis and Processing of Nanocrystalline Ceramics on a Commercial Scale”

Interdisciplinary Nanoscience Investment from University Endowment: The Harvard Center for Imaging and Mesoscale Structures (CIMS)

Harvard is making a major commitment to several areas of interdisciplinary science through the creation of several new Centers. In particular, the Faculty of Arts and Sciences has established a new Center for Imaging and Mesoscale Structures (CIMS). The emphasis of the center will be on multi-disciplinary research, bridging the disciplines of chemistry, physics, engineering, materials science, biology and medicine

The proposed initial funding for CIMS is from FAS whose main funding source is the Harvard endowment. This funding will be used for construction of new building, new major facilities and to seed new research directions. The level of funding is on the order of tens of millions of dollars and a new building. The overall aim of CIMS is to foster new interdisciplinary research on small things; the specific research areas are still under discussion but will undoubtedly include mesoscale electronics, mesoscale mechanical systems, functional nanoscale materials, and the interface between biological and physical sciences. The Center will provide space for state-of-the-art facilities (clean rooms, microscopy, synthesis - both wet and dry -, etc.), and new research space. An important point about the research space is that much of it will be assigned on a rotating basis for new interdisciplinary projects-- to provide the resources needed to pursue new directions in nanoscale research.

The length of University support of CIMS is not well defined at present. Initial plans are to provide a decreasing funding over a 10 year period with major external review after five years. This scheme is based on the desire that the researchers involved with the Center develop external funding sources (government and private) to supplement and sustain efforts. Potential partners are presently being actively pursued.

Numerous faculty members already have strong research programs in the area of nanoscience, supported in part by NIH, DoD and NSF. By providing major funds to seed and support projects and by providing world-class facilities and technical support, Harvard believes that it will create a win-win situation for academia, industry and government.

Nanotechnology Partnership: Rice University and NASA

A collaborative effort between NASA and Rice University began in October 1998 for the development of carbon nanotechnology to be used in numerous revolutionary applications. Collaborative partners with Rice in this effort are Johnson Space Center, Ames Research Center, Jet Propulsion Laboratory, and Langley Research Center. Rice is currently working on bulk production of nanotubes in a gas-phase process, suspension of tubes in a solution, and the fabrication of membranes and arrays of nanotubes that can be grown continuously. The Johnson Space Center's primary goal for nanotubes is to produce a structural material with a strength-to-weight ratio much higher than today's best composites. This work consists of production of nanotubes using electric arc and laser ablation methods, study of growth mechanisms, purification of tubes, and insertion into polymer composites for testing. Researchers from Rice have been instrumental in pushing this work forward. Preliminary work in composites has given scientists reason for optimism for eventual widespread use. These composites show promise in revolutionizing the field of materials science. The collaboration extends to Ames Research Center for modeling of the mechanical behavior of nanotubes and nanotube composites. Ames also works directly with Rice to model the high-pressure nanotube production system being developed there. The Jet Propulsion Laboratory has been involved with the nanotube effort by looking into battery and energy storage applications and is now looking further into nanoelectronics. Although the addition of Langley Research Center is relatively new, Langley is the NASA Center of Excellence for Structures and Materials. The goal of the nanotube project is to develop breakthrough technologies such as ultralightweight composites, advanced energy storage, flat panel displays, chemical sensors, nanoelectronics, and biomedical uses. These enabling technologies will help NASA achieve its missions in the new millennium. The total planned investment of NASA in the Rice collaboration is 4 to 5 million dollars over a period of five years, and Rice's contribution will be on the same order of magnitude.

Nanoscience university-industry-government investment: Northwestern University Center for Nanofabrication and Molecular Self-assembly.

A $32.5 million facility for about 140 faculty, post-doctoral researchers and graduate students is in construction on campus to provide a focal place for innovative collaborative research in applying nanotechnology to improve healthcare, environment and industrial processes. Funding comes from federal Government (Department of Health and Human Services): 14 million dollars (7 million this year, 7 million next year), private donations through Northwestern (Leo Ginger, ex-VP for R & D at Baxter Diagnostics) already has donated a million dollars, and Northwestern University that will pick up the difference. The facility is scheduled to be completed by the end of 2001. The four core research areas are developing biological structures for use in human health and industry, study solar energy conversion in order to create more efficient conversion methods, designing nanostructured polymers for electronic applications and human tissues, and using theory to predict the properties and structures for accelerating the path of discovery. The Center will build on the existing support

of $9 million per year in externally sponsored funding, including three group grants of $0.5 million each from the National Science Foundation and a block grant over five years totaling $5 million from Army Research Office for the study of atomic cluster-derived materials. Further information on the Center's mission, participants, and current research projects, is described on the website: http://www.chem.nwu.edu/NanoWeb/index.html.

Illustration of university-industry regional meetings:

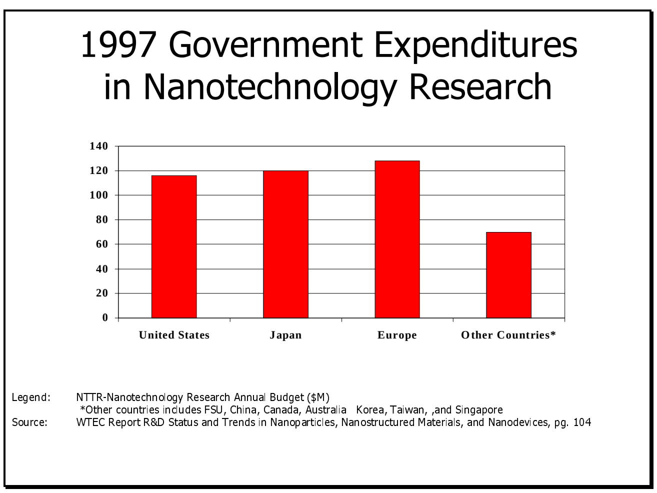
- "Minnesota Nanotechnology Summit: Opportunities and Challenges", March 17-18, 2000, Minneapolis, MN: regional meeting involving the university system and about 40 companies in the state.
- "Nanomaterial Regional Forum" sponsored by *Ben Franklin Technology Partners* (www.sep.benfranklin.org), March 30, 2000, Penn State Great Valley Campus in Malvern, PA. Objective: stimulate interaction between government agencies, key regional R&D institutions and companies, timed to support the President's 21 Jan announcement of a federal Nanotechnology Initiative. Participants Include: Government (NSF, DOE, NIH, DOD); R&D Institutions (Rutgers, Princeton, Penn State, Drexel, Penn, UDE, Fraunhofer), and area companies.
- First Georgia Tech Conference on Nanoscience and Nanotechnology, Georgia Institute of Technology, October 16 - 17, 2000 at Atlanta. Participants: Georgia Tech, Virginia Tech, University Tennessee, NC State, Duke University, Florida State University, University of Virginia, ORNL, SURA, ORAU and regional industry.

INTERNATIONAL ACTIVITIES IN NANOTECHNOLOGY

Introduction

The United States' relative strength compared with the rest of the world has changed significantly. While the United States is still the world's undisputed economic and technological leader, the world's knowledge and wealth is found in more and more locations. In 1950, the United States contributed approximately 40 percent of the developed world's GDP and carried out two to three times the total research and development (R&D) carried out by the rest of the world. By 1997, the U.S. contribution was 27 percent of world GDP, and the United States conducted about 40 percent of the world's R&D.

Nanotechnology is a prime example of the global spread of R&D. The United States, Japan and Europe all are world leaders in this area. (for further reference see "Nanostructure Science and Technology: A Worldwide Study", NSTC, 1999, (http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.Worldwide.Study/toc.htm).
While it is difficult to estimate the extent and quality of nanotechnology research taking place especially within industry, there is at least twice as much government-funded nanotechnology research going on outside of the United States as there is within it. Therefore, it is imperative the United States build international awareness and analysis, and investigates into collaborative opportunities into the National Nanotechnology Initiative from the very beginning.



The United States can be the world's leader in commercializing nanoscale devices and materials. The United States, however, is not the only nation with this capability. Many foreign countries, companies and scientists believe that nanotechnology will be the leading technology of the 21st century. They see that it has the potential to become so broad and pervasive that it will influence all areas of science, technology, and manufacturing by changing the nature of almost every human-made object. This potential, along with the fact

that there is still a chance to get in on the ground floor in this technology's development, helps explain the phenomenal levels of R&D activity worldwide.

Examples of Regional Research

The Japanese government has designed programs to establish its companies as the leaders in the development of this technology. Germany and the United Kingdom have programs comparable in scale and sophistication to Japan, but with differences in research emphasis. China also is undertaking major efforts in nanotechnology. Other major players are Australia, France, India, Taiwan, Korea, Singapore, Russia, Switzerland, and Canada. It is essential, therefore, to be able to transcend geographic location to understand and craft this technology.

Japan

The Japanese Government spent about $120 million on nanotechnology research in 1997. It has significant capital infrastructure for nanotechnology in its national laboratories, universities and companies. The quality of its science in this area is high, it has ample human resources and has a large number of first-class collaborations among national laboratories, academic institutions and company researchers. Government and very large corporations are the main sources of funding for nanotechnology in Japan. Japan is attempting in the relatively new field of nanotechnology to provide an opportunity for researchers to become more proactive and less traditional. Japanese research centers around three main areas: quantum functional devices, biotechnology, and smart materials. Appendix One lists major Japanese centers of excellence and projects on nanotechnology and, if available, the approximate amount they spend per year.

Western Europe

In Europe, there is a combination of national programs, collaborative European Union projects and networks, and large corporations investing in nanotechnology. The United Kingdom, Germany and France all have major national programs and capabilities in nanotechnology. Researchers in other countries such as the Netherlands and Switzerland also are doing significant work. European Government Expenditures on nanotechnology were about $128 million in 1997.

The European Union's Fifth Framework Program will run for four years and began at the end of 1998. It continues work already begun on nanotechnology in previous R&D programs, and added a new emphasis on nano-biology. The European Union's ESPRIT Advanced Research Initiative in Microelectronics and the BRITE/EURAM projects on materials science both are partially dedicated to nanotechnology. The PHANTHOM (Physics and Technology Mesoscale Systems) is a network with about 40 members created in 1992 in order to stimulate nano-electronics, nanofabrication, opto-electronics, and electronic switching. The European Science Foundation sponsors NANO to promote collaboration between the aerosol and materials science communities on nano-particles. Other major European programs that are: NEOME (Network for Excellence on Organic Materials for Electronics); the European Society

for Precision Engineering and Nanotechnology, and the Joint Research Center Nanostructured Materials Network.

The German Federal Ministry of Education and Research (BMBF) spends approximately $50 million per year on nanotechnology. BMBF is supporting precompetitive R&D projects in nanotechnology with a plan to scale-up spending over the next few years. Areas of emphasis include: nanoanalysis, ultrathin films, lateral nanostructures, nanomaterials, and ultraprecision engineering. In 1998, it began an initiative to fund six competence centers as a platform for the accelerated development of nanotechnology. The goal of these centers is to bring together science, economics and venture capital to quickly spread information and results, coordinate an educational effort, and stimulate the formation of start-up companies.

The British Government created the LINK Nanotechnology Programme in 1988 with an annual budget of about $2 million. The Engineering and Physical Sciences Research Council funded $7 million worth of materials science projects related to nanotechnology from 1994-1999, and plans to continue funding this area. The National Physical Laboratory established the National Initiative on Nanotechnology to promote nanotechnology in universities, industry, and government. In addition, some British universities, such as Oxford University, conduct leading edge nanotechnology research.

Other Examples

- Singapore has a national program initiated in 1995.
- Australia's National Research Council sponsors significant amounts of nanotechnology R&D. There are also programs in Australian universities and industry.
- Korea has included nanotechnology as a national focus area since 1995 and is in the process of establishing a special research center on nanoscale semiconductor devices.
- Taiwan is increasing nanotechnology research through the Industrial Technology research Institute and its National Science Council to ensure it can retain a leading position in information technology.
- China is just completing a ten-year nanotechnology program "Climbing Project on Nanometer Science" and plans major new activities. It also has significant relevant research on advanced materials, nanoprobes and manufacturing processes using nanotubes.
- Russia has established the Russian Society of Scanning Probe Microscopy and Nanotechnology, and has particular strengths in preparation processes of nanostructured materials and nanocrystalline structures.

List of Japanese Centers of Excellence and Major Funders in 1997

Ministry of International Trade and Industry ($60 million)*

- National Institute for Advancement of Interdisciplinary Research ($28 million)
- Electrotechnical Laboratory ($17 million)
- Osaka National Research Institute ($3 million)
- National Industrial Research Institute of Nagoya ($2.5 million)
- Quantum Functional Devices Program ($6.4 million)
- Ultimate Manipulation of Atoms and Molecules Program ($25 million)
- Frontier Carbon Technology Program ($15 million)
- Smart Materials Program ($9 million)
- Optical Disk Systems with Nano-Precision Control Program ($12 million)
- Super Metal Technology Program ($10 million)

*Subtotals are higher than total MITI funding because some Programs listed do not clearly delineate nanotechnology research.

Science and Technology Agency ($35 million)

- Institute of Physical and Chemical Research, Frontier Materials Research
- National Research Institute for Metals
- Core Research for Evolutional Science and Technology (CREST) Projects
  - --Quantum Devices
  - --Single Atomic and Molecular Manipulations
- Japan Science and Technology Corporation's ERATO Projects
  - --Quantum Wave Project
  - --Atomcraft Project
  - --Electron Wavefront Project
  - --Quantum Fluctuation Project

Ministry of Education, Sports and Culture

- Tokyo University
  - --Research Center for Advanced Science and Technology
  - --Institute of Industrial Engineering
  - --Chemical Engineering
- Kyoto University
- Tokyo Institute of Technology, Bioelectric Devices
- Tohoku University, Institute of Materials Science
- Nagoya University
- Osaka University
- Institute of Molecular Science
- Exploratory Research on Novel Artificial Materials and Substances for Next Generation Industries

Industry

- Hitachi Central R&D Laboratory
- NEC Fundamental Research Labs
- Toshiba Research Center
- Nihon Shinko Gijutsu (ULVAC)
- NTT
- Fujitsu
- Sony
- Fuji Photo Film Company

NATIONAL NANOTECHNOLOGY INITIATIVE PUBLICATIONS

Below is a list of nanotechnology publications that have been prepared by the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee (formerly IWGN) of the National Science and Technology Council's Committee on Technology.

Nanotechnology: Shaping the World Atom by Atom

(http://www.nano.gov or
http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.Public.Brochure/welcome.htm).

This glossy publication sets the stage for increasing the public's understanding of what nanotechnology is, how nanotechnology came to be, and its potential impact on society. "The emerging fields of nanoscience and nanoengineering are leading to unprecedented understanding and control over the fundamental building blocks of all physical thinks. This is likely to change the way almost everything – from vaccines to computers to automobile tires to objects not yet imagined – is designed and made."

National Nanotechnology Initiative – Leading to the Next Industrial Revolution

(http://www.nano.gov or
http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.FY01BudSuppl/toc.htm)

This report supplements the President's FY 2001 Budget and highlights the nanotechnology funding mechanisms developed for this new initiative as well as the funding allocations by each participating Federal agency. This report unveils the President's bold, new initiative coordinating focussed areas of research and development (R&D) among the Federal government, academia and university to advancing nanotechnology.

Nanostructure Science and Technology: A Worldwide Study
(http:///www.nano.gov/ or
http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.Worldwide.Study/toc.htm).

This report reviews the status of R&D in nanoparticles, nanostructured materials, and nanodevices, including innovative approaches to synthesis and characterization. The report highlights applications in dispersions, high-surface area materials, electronic and magnetic devices, nanostructured materials, and biological systems. It includes a comparative review of research programs around the world – the United States, Japan, Western Europe, and other countries – to help provide a global picture of the field.

IWGN Workshop Report: Nanotechnology Research Directions

(http://www.nano.gov/ or
http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.Research.Directions/toc.htm)

This publication builds upon *Nanostructure Science and Technology: A Worldwide Study* (http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.Worldwide.Study/toc.htm), and incorporates a vision for how the nanotechnology community -- Federal agencies, industries, universities, and professional societies -- can more effectively coordinate efforts to develop a wide range of revolutionary commercial applications. *Nanotechnology Research Directions* identifies challenges and opportunities in the nanotechnology field and begins to make recommendations on how to develop a balanced R&D nanotechnology infrastructure, advance critical research areas, and nurture the scientific and technical workforce of the next century. It incorporates perspectives developed at a January 1999 IWGN-sponsored workshop by experts from universities, industry, and the Federal government.

President's Committee of Advisors on Science and Technology Endorsement to the President

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EXECUTIVE OFFICE OF THE PRESIDENT
PRESIDENT'S COMMITTEE OF ADVISORS ON SCIENCE AND TECHNOLOGY
WASHINGTON, D.C. 20502

December 14, 1999

The President of the United States
The White House
Washington, DC 20500

Dear Mr. President:

Your Committee of Advisors on Science and Technology (PCAST) strongly endorses the establishment of a National Nanotechnology Initiative (NNI), beginning in Fiscal Year 2001, as proposed by the National Science and Technology Council (NSTC). Our endorsement is based on a technical and budgetary review of a comprehensive report prepared by the NSTC Committee on Technology's Interagency Working Group on Nanoscience, Engineering and Technology (IWGN).

We believe that the Administration should make the NNI a top priority. America's continued economic leadership and national security in the 21st century will require a significant, sustained increase in nanotechnology R&D over the next 10 to 20 years. We strongly endorse the robust funding and the research strategy that has been proposed by the NSTC's IWGN.

Nanotechnology is the science and engineering of assembling materials and components atom by atom, or molecule by molecule, and integrating them into useful devices. It uses new discoveries, new eyes (high resolution microscopes) and hands (laser tweezers) to work, at the scale of a nanometer (one billionth of a meter – ten thousand times smaller than the diameter of a human hair).

Nanotechnology thrives from modern advances in chemistry, physics, biology, engineering, and materials research. We believe that nanotechnology will have a profound impact on our economy and society in the early 21st century, perhaps comparable to that of information technology or of cellular, genetic, and molecular biology. Nanotechnology also promotes the convergence of biological, chemical, materials and physical sciences and engineering disciplines.

Nanotechnology is the first economically important revolution in science and technology (S&T) since World War II that the United States has not entered with a commanding lead. Federal and industrial support of R&D in the United States for this field already is significant, but Europe and Japan are each making greater investments than the United States is, generally in carefully focused programs. Now is the time to act.

In our view, the Federal government, together with academia and industry, plays a vital role in advancing nanotechnology. This role will require a new, bold national initiative coordinating focused R&D in the decade ahead. Today nanoscale S&T is roughly where the fundamental R&D on which transistors are based was in the late 1940s or early 1950s. Most of the work currently required is still fundamental, with a much longer time horizon than what most industries can support. The NNI is balanced well across fundamental research, grand challenges, centers and networks of excellence, research infrastructure, and education and training.

We believe that the science, technology, applications, products, and programs catalyzed by the NNI will inspire a new generation of young Americans with exciting new opportunities and draw them to careers in S&T. Potentially the NNI will help provide for a better world through advances in environmental technologies, lowering of energy consumption, and advances in medical diagnostics and therapeutics.

The NNI is an excellent multi-agency framework to ensure U.S. leadership in this emerging field that will be essential for economic and national security leadership in the first half of the next century. We recommend that progress toward NNI goals be monitored annually by an appropriate external body of experts, such as the National Research Council.

A brief summary of our review of the IWGN report, National Nanotechnology Initiative – Leading to the Next Industrial Revolution, is enclosed. We hope that our recommendations will be helpful as you consider your priorities for Federal investments.

We look forward to discussing this review with you, with members of your Administration, and with members of Congress.

Sincerely,

Neal Lane	John Young
Co -Chair	Co-Chair

PRESIDENT'S COMMITTEE OF ADVISORS
ON SCIENCE AND TECHNOLOGY
PANEL ON NANOTECHNOLOGY
REVIEW OF PROPOSED NATIONAL NANOTECHNOLOGY INITIATIVE
NOVEMBER 1999

Summary
PCAST believes that the benefits to the United States of the National Nanotechnology Initiative (NNI) are compelling, and we endorse the funding level, balance, and mechanism recommended by Interagency Working Group on Nanoscience, Engineering and Technology (IWGN).

Our Review
A PCAST Nanotechnology Panel, composed of industry and university experts and chaired by Dr. Charles Vest, carefully reviewed the report entitled National Nanotechnology Initiative – Leading to the Next Industrial Revolution, written by the National Science and Technical Council (NSTC) Committee on Technology's Interagency Working Group on Nanoscience, Engineering and Technology (IWGN). This report frames a new interagency R&D initiative, the NNI, starting in Fiscal Year 2001, and proposes a 5-year funding plan, appropriately distributed across both agencies and funding mechanisms. The NNI has an essential exploratory and scientific component and focuses on fundamental aspects of nanoscale science and engineering that collectively have high potential to eventually lead to important applications, processes, and products. These outcomes will strengthen both scientific disciplines and create critical interdisciplinary opportunities. Our Panel reviewed the technical merits and the funding profiles in the NNI proposal and supports the IWGN recommendation for a substantial budget increase in Fiscal Year 2001 with sustained funding in this area.

The NNI research portfolio is balanced well across fundamental research, Grand Challenges, centers and networks of excellence, research infrastructure, and education and training. The NNI also provides mechanisms for building workforce skills necessary for future industrial and academic positions, proposes cross-disciplinary networks and partnerships, includes a mechanism for disseminating information, and suggests tools for encouraging small businesses to exploit nanotechnology opportunities. If it is implemented, we recommend that the NNI be annually reviewed by a non-government advisory committee, such as the National Research Council, to monitor and assess progress toward its goals.

Nanotechnology is the future.
Nanotechnology is the builder's new frontier – one where properties and phenomena are very different than those utilized in traditional technologies. Nature builds things with atomic precision. Every living cell is filled with natural nanomachines of DNA, RNA, proteins, etc., which interact to produce tissues and organs. Humans are now learning to build non-biological materials and machines on the nanometer scale, imitating the elegance and economy of nature. This embryonic capability may portend a new industrial revolution. In the coming decades, nanotechnology will enable us to manufacture devices that conduct electricity efficiently, compute, move, sense their environment, and repair themselves.

Nanostructures will revolutionize materials and devices of all sorts, particularly in nanoelectronics and computer technology, medicine and health, biotechnology and agriculture, as well as national security. For example, we anticipate computers with a thousand-fold increase in power but which draw a millionth the amount of electricity, materials far stronger than steel but with ten percent the weight, and devices that can detect tumors when they are only clusters of a few cells.

It may eventually be possible to develop technologies for renewable, clean energy; to replace metals with lightweight, recyclable polymeric nanocomposites; to provide low-cost access to space; and to develop new classes of pharmaceuticals. Investments in nanotechnology have the potential to spawn the growth of future industrial productivity. When allied with the biosciences, nanotechnology will accelerate the development of early detection instruments for physicians, as well as the development of noninvasive diagnosis and medical treatment. It will also lower the cost of pure water and healthy food for the world's population.

The United States cannot afford to be in second place in this endeavor. The country that leads in discovery and implementation of nanotechnology will have great advantage in the economic and military scene for many decades to come.

A bold, Federally funded national program is needed now.
Nanotechnology, which is based on phenomena first observed and characterized in the 1980s, is now emerging as an important new frontier. Direct, strategic investments made now in fundamental science and engineering will position the U.S. science and technology (S&T) community to discover and apply nanoscale phenomena, and transfer them to industry. Nanoscale S&T today is roughly where the fundamental R&D on which transistors are based was in the late 1940s or early 1950s. Most foreseeable applications are still 10 or 20 years away from a commercially significant market; however, industry generally invests only in developing cost-competitive products in the 3 to 5 year timeframe. It is difficult for industry management to justify to their shareholders the large investments in long-term, fundamental research needed to make nanotechnology-based products possible. Furthermore, the highly interdisciplinary nature of some of the needed research is incompatible with many current corporate structures.

There is a clear need for Federal support at this time. Appropriately, Federal and academic investments in nanotechnology R&D to date have evolved in open competition with other research topics, resulting in some fragmentation and duplication of efforts, which is natural at this stage. Going forward, however, nanotechnology will require a somewhat more coherent, sustained investment in long-term research. The NNI would support critical segments of this research and increase the national infrastructure necessary to conduct it.

International Activity in Nanotechnology
The United States does not dominate nanotechnology research. Yet we strongly believe that the United States must lead in this area to ensure economic and national security leadership. Compared to our nation, other countries are investing much more in relevant areas of ongoing research. Many other countries have launched major initiatives in this area, because their scientists and national leaders have determined that nanotechnology has the potential to be a major economic factor during the next several decades. Japan and Europe are supporting scientific work of the same quality and breadth of that done in the United States. Unlike in the other post-war technological revolutions, the United States does not enjoy an early lead in nanotechnology.

We must act now to put in place an infrastructure for nanoscale research that is equal to that which exists anywhere in the world. A suitable U.S. infrastructure will enable us to collaborate appropriately, as well as compete, with other nations. Without the NNI, there is a real danger that our nation could fall behind other countries. To ensure leadership in the future, the United States must make a large and sustained investment in this area.

Nanotechnology will inspire the public and the next generation workforce.
Our future workforce in S&T is decreasing, in part because far too many young people perceive that action is no longer in the physical sciences and engineering, and do not see how S&T connects to the world as they know it. Yet chemistry, physics, biology, engineering, and materials research are at the core of nanotechnology, which likely will play a dominant role in future decades. The NNI should parallel

investments in R&D with a creative and entrepreneurial program that offers young people a truly interdisciplinary education, and that prepares the next generation of researchers and industrial leaders.

As nanotechnology develops, the core areas of the physical sciences, engineering and biomedicine in our nation's universities will become much more intimately coupled to each other. Future research efforts in these fields need a far better integration among each other and to industry and society as a whole. The relevance and inherent excitement of nanoscale R&D should attract young men and women to science as never before and also create exciting and important career options for them.

Nanotechnology and Global Challenges

In the next century, the world population will likely grow to over ten billion. Without revolutionary advances in environmentally sustainable technologies, global society will struggle with the implications of this growth. Nanotechnology, as broadly supported by the NNI, has the potential to develop lightweight, recyclable materials and energy efficient devices that will contribute to such sustainability. Therefore, the United States should move to develop this area quickly, not only for economic benefit, but also for its potential contribution to a more sustainable future.

In closing, we note that when radically new technologies are developed, social and ethical issues can arise. Accordingly, we recommend that a modest amount be set aside for the study of such implications of nanotechnology.

Agencies' Contributions to FY 2001 NNI Implementation Plan and to NSET Subcommittee Activities

(DOC, DOD, DOE, DOT, NASA, NIH, NSF)

D1. Department of Commerce (DOC/NIST)

a. Background

NIST's fundamental mission is to support U.S. industry with the measurements, standard materials and data needed for global competitiveness and to ensure continued economic growth. NIST is the only organization that has the mission and the necessary combination of staff expertise, experience, industry contacts, industry respect, and worldwide recognition as the leading measurement and standards institution. NIST has unique experience in working with the breadth of industries impacted by nanotechnology, from electronics to biotechnology. Research into such measurement areas as quantum electron counters for high accuracy electrical calibrations, giant magnetoresistance for magnetic data recording, DNA diagnostics for health care, and atomic scale imaging and spectroscopies for semiconductor technology has made NIST a world leader in nanotechnology. NIST staff expertise in materials, electronics, physics, chemistry, and manufacturing technology makes NIST uniquely qualified to address the high risk scientific and technological challenges associated with developing the measurement techniques and technical standards needed in this new field.

b. Investment Strategy

At the proposed funding level, NIST will develop the critical enabling infrastructural measurement, standards and data in the areas of nanodevices, nanomagnetics, nanomanipulation, and nanocharacterization.

Nanodevices: NIST will develop measurements, standards and data for the nanotechnology industry using the evolving "top-down" approach, including the semiconductor, communications, and health care industries. "Top-down" technologies evolve over the years from large centimeter scales down to smaller and smaller dimensions until they reach nanoscale dimensions. NIST will also use this approach to develop new measurement techniques and methods. This focus will allow NIST to meet the short- to medium-term needs of U.S. industry. NIST proposes the following areas of nanodevice research:

- NIST will develop a suite of quantum standards that attain near absolute accuracy for exact calibration of physical parameters (e.g., electrical, mass, force, and chemical analysis.)
- NIST will develop measurements, standards and data that support the use of new semiconductor processing and manufacturing approaches, including: standard data to support deep UV and X-ray lithographic methods; measurement techniques to determine the effectiveness of plasma processing and rapid thermal processing; X-ray optics and single-ion etching/lithography; and a variety of dimensional, electrical, chemical, nanoparticle contamination, and other standard

materials that will be made to meet the rising demand from the semiconductor manufacturing industry.

- Nanoscale versions of table-top analysis instruments, frequently referred to as “lab-on-a-chip” technology, promise to revolutionize many chemical and physical measurements with wide ranging applications in health care, environmental, and industrial process monitoring. These devices will move many laboratory measurements into the field, e.g., to the doctor's office or the plant floor. NIST will develop measurements and standards supporting this growing technology area, including dimensional, chemical, and electrical standards that are needed to assure the quality of results from these devices. The masses and volumes measured by these devices are much smaller than previously attained and NIST will need to develop methods to make standards that are homogeneous at the nanoscale level, a new requirement for many of our standard materials.

Nanomanipulation: “Bottom-up” nanomanufacturing – building useful objects from single atoms or molecules – is based on the ability to manipulate nanoscale particles. The “bottom-up” synthetic approach uses nanomanipulation to develop nanomaterials and devices- such as self-assembled monolayers and multilayers and scanning probe manipulators- from atomic and molecular scale manipulation. This initiative in nanomanipulation will include the following areas:

- To achieve high volume production in nanoscale manufacturing, it will be necessary to mimic nature’s strategy of self-assembly and self-replication. Progress in the area of self-assembly of thin films is being made; however, better measurements of the forces governing self-assembly are needed to enable assembly of the complex structures desired for catalysis, sensing, molecular separations, biomaterials, and molecular electronic devices. NIST will develop standards for autonomous atom assembly to permit detailed measurement of their physical, electronic and magnetic properties.
- Many manufacturing processes can be controlled and manipulated in more accurate and novel ways if we understand the mechanics of nanoscale systems, including nanofluidics and nanoparticulates. NIST will develop single particle tracking, manipulation, and measurement methods for investigation of molecular transport in biological, bio-mimetic, and bio-engineered metallic oxide films and membranes and other manufacturing processes.
- A great challenge for computational research is the accurate and reliable estimation of the properties, reactivity, and bulk behavior of molecules in the condensed phase, including solutions, surfaces, solids, and interfaces. NIST will integrate first-principles, predictive quantum methods with atomistic statistical methods for sampling configurations and properties at finite temperature and pressure. To date, this has been accomplished for only the simplest systems. This capability will supercede current empirical methods and simplistic models. Many roadmaps and workshops have highlighted the need for work in this important area from the point of view of process and product design in the 21st century.

Nanocharacterization: Tools for visualization and characterization are vital to understanding nanotechnology. Measurement and characterization at the nanoscale are necessary to understand the nature of nanomanufacturing processes, to assess the purity of nanoscale products and components, and to understand mechanisms of interaction of the product with its environment, including failure during operation. Industry requires a new set of characterization tools and standards since existing characterization approaches and standards are insufficient, lacking the

necessary spatial resolution or specificity needed for nanotechnology. Industry cannot successfully make nanodevices or components until they can be accurately measured and characterized. NIST will develop measurement methods and standards that allow atomic scale resolution in three dimensions with accurate physical and chemical functional specificity. NIST proposes:

- To develop smart measurement probes sensitive to electronic, magnetic, chemical or biological properties, e.g., a nano-tip including a single electron transistor for ultra-sensitive charge measurements, a superconductor tip for electron spin detection, or chemically/biologically functionalized tips for nanoscale analysis to support semiconductor, chemical and materials processing, pollution monitoring, medical diagnosis, and food quality control. The weak link in such measurements has always been the specificity of the detection material. The recent development of molecularly-tailored nanostructures composed of metals, semiconductors, polymers, or DNA opens exciting new opportunities for sensing. NIST will develop both new sensors and the electrical and optical measurement methods to enable the use of these chemically and physically selective nanomaterials in measurement devices. These new probes will allow NIST to support the increasing use by industry of combinatorial approaches to materials characterization and synthesis.
- To develop measurement instrumentation and the theoretical basis for interpreting images and analyses including the quantitative 3-D measurement methods to allow accurate interpretation of chemical, physical, and dimensional data from these new technologies, neutron and x-ray reflectometry, small angle scattering, and spectroscopic analysis, and standard materials and data. The techniques of microscopy and nanoanalysis based upon beams of electrons, ions, photons, neutrons and scanned probes are key assets in the nanotechnology fields.

Nanomagnetics: The magnetic data storage industry is an example of the widespread commercialization of nanotechnology. Magnetic storage bits on new computer hard disks currently measure 80 nanometers by 500 nanometers, and read/write head flying distances are only 20 nanometers. The trend in information storage continues toward higher information density and higher access speed, both of which double every two to three years. Many problems and challenges face the magnetic information storage industry at this especially critical time. NIST proposes to work in the following areas:

- Magnetic Bit Stability and Kinetics in Thin Films. NIST will develop ultra-high-speed measurements of magnetization dynamics for characterization of speed capabilities of thin film materials to support gigabyte storage. At the other extreme is the need for multi-year stability of a bit once it is written, despite thermal fluctuations, which can degrade very small-area bits. Measurements and models will be developed to meet these industrial needs.
- Imaging Methods for Nanomagnetics. With recording bits having sizes as small as 250 by 25 nanometers, being able to image possibly misaligned magnetic structures as they are recorded is a critical capability for design engineers. NIST will realize this measurement capability with the development and application of a microscope which uses electron spin and other methods to image magnetic domains.
- Physical Standards for Magnetic Measurements. New standards are needed by industry for measurements on read/write heads and magnetic disks. This project will produce standards for films having a magnetic moment 100,000 times smaller than references now available from NIST.

Also, as nanotechnology is a broad field with diverse industry needs, NIST will leverage our efforts to efficiently and effectively meet the measurement and standards needs of U.S. industry while maintaining our institutional flexibility and responsiveness to rapidly changing customer needs. NIST will develop stronger strategic alliances/collaborations with universities, businesses and other government agencies that possess leading expertise in nanotechnology to conduct much of the specific work required to meet the goals of this initiative and avoid developing costly, complex in-house capabilities that will be used only once. The university alliances will also help educate the U.S. workforce in nanotechnology related problems, and permit NIST scientists and engineers to concentrate on the critically needed metrology and research, while contracting out development of specific equipment and techniques. Building these partnerships will return greater value to the taxpayers for their investment in nanotechnology.

Because nanotechnology is in its initial stages of discovery and growth, many effects cannot be imagined let alone accurately predicted. NIST predicts that this technology will have a major effect on every industrial sector. This new technology area requires a large infrastructure to aid rapid U.S. commercialization of new discoveries. A major contribution to that infrastructure is NIST-based measurements, standards and data that industry must use to see if and how well their products work.

Table D1. NIST NNI Summary

Nanotechnology Initiative	
Technical Area	Outputs
Nanodevices	• Develop two new standard reference materials for semiconductor, lab-on-a-chip, and other nanotechnologies • Develop new quantitative measurement methods for analysis of physical and chemical properties of industrial nanoscale devices such as semiconductors • Publish papers on the development of measurement methods, standard reference materials, and calibration systems.
Nanomanipulation	• Develop standards for autonomous atom assembly. • Develop modeling and simulation programs for condensed phases, including solutions, surfaces, solids, and interfaces • Publish papers on the development of manipulation and modeling data, algorithms, and related research.
Nanocharacterization	• Develop three new standard reference materials for calibration and quality assurance of commercial analysis laboratories and instruments. • Develop several 3-D measurement methods for the analysis of physical and chemical at or near atomic spatial resolution. • Publish papers on the development of measurement methods and standard reference materials.
Nanomagnetics	• Develop stability and kinetics measurement systems and standard data for magnetic thin films. • Develop two new standard reference materials. • Publish NIST papers and university partnership papers on the measurements and standard reference materials for magnetic data storage.

D2. Department of Defense (DOD)

a. Background

The DOD basic research effort is intended to enable revolutionary new capabilities of importance to the DOD and the Nation. DOD's priorities are aligned with the Basic Research Plan, with the OSD guidance for basic research, and with the Joint Vision 2010, the Chairman of the Joint Chiefs' conceptual template for achieving new levels of warfighting effectiveness. These documents forecast dynamic change in the nature of potential adversaries and emphasize the increasingly critical nature of technological advances.

The Director, Defense Research and Engineering (DDR&E) identified "nanoscience" as one of six strategic research areas (SRA) in 1996. The Nanoscience SRA is formally coordinated by a committee comprised of four members, one from each service and DARPA, with a rotating chairperson. In addition to the formal members, the Nanoscience SRA committee routinely queries scientific officers from the various DOD funding agencies and principal investigators for the DOD laboratories. The DOD funding agency nanotechnology topics/programs are identified in Table D2.1; they represent the several disciplines that will be necessary to enable the interdisciplinary programs demanded in the NNI. In addition, the DOD laboratories have programs establishing the nanoscience base necessary to develop innovative technologies to meet DOD needs. The principal DOD laboratory science and technology areas are listed in Table D2.2.

Table D2.1 DOD Funding Agency Nanotechnology Interests

<u>Biology</u>	
AFOSR	Nanobiomimetics; Nanosensors for IR
ARO	Nanobiotechnology
ONR	Molecular motors and actuators in NEMS; Marine nanostructure assembly mechanisms; Nanostructures in biomolecular recognition
<u>Chemistry</u>	
AFOSR	Organic Nanostructures, Molecular electronics, Nanocomposites; Nanostructured Catalysis; Cluster based materials
ARO	Surface/Interface Chemistry; Nanocomposites/energetic materials
ONR	Molecular Electronics, Nanotubes, NEMs, and Self Assembly; Nanostructures in Electrochemical Systems; Molecular Electronics, Nanotubes
<u>Electronics</u>	
AFOSR	Radiation effects on nanostructures, Terahertz; High-density memory devices, distributed nanosensors
ARO	Solid State Devices; High Frequency Electronics
DARPA	Molecular Electronics, Molecular-level Printing, NEMS; Advanced Lithography; Nano-scale electronic devices and circuits
ONR	Nanoelectronic Physics, Devices, Circuits; Nano-magnetics, Bioelectronics; Fabrication
<u>Materials</u>	
AFOSR	Fabrication of nanoscale structures
ARO	Physical Behavior of Nanomaterials
ONR	Nanostructured Materials/Coatings
<u>Physics</u>	
AFOSR	Nanoscience, Quantum Structures & Computing
ARO	Interface/Surface Physics, Molecular Machines; Nanoscience, Quantum Information Physics
DARPA	Spin Electronics; Quantum Information Processing

Table D2.2 DOD Laboratory Nanotechnology Science and Technology Areas

Biology	
ARL	Nanobiodetection
AFRL	Nanobiomimetics
NRL	Nanobiochemistry, Biosensing, NEMS; Nanobiomaterials
Chemistry	
AFRL	Self assembly; Nanoscale energetic materials
NRL	Nanochemistry, Proximal Probe Sensing; Nanowires; Cluster Chemistry/Assembly
Electronics	
AFRL	Nanoelectronics; Molecular computing; nanostructure theory; Magnetic Nanoparticles
AFRL/SNH	Matter-wave Nanolithography; Quantum Dots for Hyperspectral Devices; Terahertz
ARL	Quantum dot; Quantum Well IR Sensors; Semiconductor nanostructures; Semiconductor nanostructures; VCSELS, quantum optics
NRL	Nanofabrication; Quantum Dots; Nanoelectronic Physics; Nanoelectronic Physics; Quantum Device Physics and Networks; Magnetic Nanostructures on Semiconductors
CECOM	Stability/Noise of NEMS; RF NEMS
Materials	
AFRL	Carbon-based nanotubes/foams; nanocomposites; Nanostructures for composites; Nanostructured materials, Nanocomposites, Polymeric Nanofabrication; Multiscale computer simulations; Nanophase metal and ceramics
AFRL/SNH	Materials for nanoscale device structures
NRL	Multifunctional Nanostructured Coatings
SBCCOM	Nanomaterials
ARL	Nanomaterials, nanobiotechnology
Physics	
AFRL	Nanostructured optical materials; Nanotribology; Nano-structured Optical materials; simulations
AFRL/SNH	Nanostructures in Quantum Computing and Communications
ARL	Mesophysics; Nanophysics; Subwavelength optics, photonic bandgap; Quantum information science
AMCOM	Quantum information science, photonic bandgap
NRL	Carbon Nanotube Theory; Magnetic Interfaces/nanostructures; Quantum Dot Optics; Optical Spectroscopy of Nanostructures; Nanomechanics

Each DOD SRA is reviewed biannually during the DOD Technical Area Requirements and Assessment. This review examines the investment strategy for the SRA with special attention to the goal of transitioning new ideas stemming from the SRA basic research investment into DOD applied research and development programs. The program is evaluated with attention to the DOD needs and interests. Metrics for SRA scientific success include: refereed journal articles, invited talks to professional conferences, and professional science/engineering society awards -- all accepted evidence for intellectual prowess. The NNI is so named to call attention to the importance of transitioning intellectual advances into commercial technologies. The 5-year time frame of the NNI is too short to expect extensive transition of research findings into full-blown technology. However, there are several metrics to identify successful steps toward this goal: creation of funded DOD programs in applied research (6.2) and exploratory development (6.3) based on the basic research discoveries; patented ideas, especially with licenses to demonstrate commercial interest;

citation of journal results in other patents; and cooperative research and development agreements (CRDAs) with industry. All these metrics will be used to evaluate the success of the NNI funded programs.

The nanometer science SRA presently has a $70M/yr investment. As a basic research investment, the program has focussed on accelerating progress in nanoscience by attending to:

	FY00
Fabrication, synthesis and processing	$37M
Nanoscale characterization	$ 2
Novel phenomena/properties	$18
Nanodevice concepts	$13
Total	$70 M

DOD participation in NNI is coordinated by the Research Director in the Office of Director, Defense Research and Engineering (DDR&E), whose primary responsibility is to manage a research investment that will maintain US technological superiority over potential adversaries. Both the Research Director and the Chair of the DOD Nanoscience Strategic Research Area are members of the NSET Subcommittee.

b. Investment Strategy

The NNI research portfolio (page 27, National Nanotechnology Initiative, supplement to the President's FY2001 Budget) identifies the DOD research investment as:

	Total	Plus-up
Fundamental Research	$10 M	$ 4 M
Grand Challenge	54	23
Centers/Networks	24	8
Research Infrastructure	19	5
Societal Implication/Workforce	3	0
Total	110 M	40 M

The NNI provides a $40M augmentation to the existing SRA program. Those funds have been allocated to two separate budget lines:

$30M	DDR&E URI	OSD 601103D
$10M	Navy Basic Research	Navy 601153N

This breakout was chosen consonant with the goal of providing approximately 75% of the research funding to University investigators; the OSD URI budget line can fund only university research. Since a goal of the NNI is augmented collaboration amongst university/industry/government, the ONR budget line is available so that DOD laboratories and industry can participate.

As a mission oriented agency, the DOD views both its investment in Fundamental Research and Grand Challenges as providing the science base necessary to accelerate progress toward technologies assisting the Defense mission. Three of the NNI Grand Challenge topic specifically identify a leading DOD role: Bio-nanosensor Devices for Communicable Disease and Biological Threat Detection; Nanostructured Materials “by Design”; and Nano-Electronics, Optoelectronics and Magnetics. Note that the NNI headings Centers/Networks, Research Infrastructure, and Societal Implication/Workforce are funding mechanisms and can also be cost allocated against research topics. The present SRA investment can be cast in terms of the NNI grand challenges that rely on DOD leadership:

	FY00
Nanoelectronics, optoelectronics, magnetics	$53M
Nanomaterials…	15
Bionanodevices…	2
Total	$70M

The NNI funding for the DOD will largely be utilized to augment programs in these three grand challenges. The distribution of DOD augmented funds between these three challenges will be determined by the collaborations with other NSET agencies (principally DOE, NASA in nanoelectronics; NSF, DOE in nanomaterials; and NSF, NIH, DOE, NASA in nanobiotechnology) and the quality of proposals received. However, it is anticipated that there will be better balance amongst the funding levels of the three challenges.

DDR&E organized a planning meeting to determine the most advantageous approaches for investing the $30M URI funds that must go to Universities. Prior to the planning meeting, the service/DARPA scientific officers and principal investigators in nanoscience debated the various investment opportunities. The planning meeting, held on March 16, included participants from other NSET Subcommittee (NSF, DOE, NIH) so that greater cooperation/collaboration between agencies can be achieved in the NNI. Approximately $15-20M of the FY01 plus-up in the URI will be competed in a Defense University Research Initiative on Nanotechnology (DURINT) which will run in parallel with the annual DOD MURI competition. The DURINT will focus attention on multidisciplinary projects, an aspect critical to rapid progress and innovation at the nanoscale. DOD laboratory participation in the University proposals to DURINT will be encouraged. Approximately $10-15M of the FY01 plus-up will be competed as equipment or fellowship grants to Universities. These latter competitions will not commit any resources beyond the FY01 allocation, thereby enabling flexibility for new commitments in the succeeding years of the NNI. At present the DOD funding is flat across the five year NNI program. Given the rapid progress in the science of nanostructures, the out-year flexibility is essential to an intelligent investment strategy. There will also be programs to invest in DOD laboratory programs and infrastructure. The NNI, like all DOD S&T programs, will have funds distributed on the basis of competitions with the best ideas selected.

The DOD has been working with the other NSET Subcommittee members to ensure the most effective investments in nanoscience. DOD participated in the NIH planning for the Bioengineering Consortia (BECON) symposium on Nanoscience and Nanotechnology Shaping Biomedical

Research. Since NIH has far greater resources than the in biology/medicine, the DOD investment in nanobiotechnology must be closely coordinated with NIH. DOD has also been working with NSF on a potential simulation/modeling effort that would complement the recent BAA announcement NSF 00-36 “Nanoscale Modeling and Simulation”; the historical DOD attention to high performance computing makes this opportunity particularly promising.

D3. Department of Energy (DOE)

a. Background

Nanoscale Science, Engineering, and Technology Research (NSET) is the contribution to the National Nanotechnology Initiative -- Leading to the Next Industrial Revolution (NNI) of the Basic Energy Sciences (BES) Program of the Office of Science (SC), U.S. Department of Energy (DOE). This document provides a summary of the program description and implementation plan for BES.

Controlling and manipulating matter at the atomic and molecular scale is the essence of nanoscale science, engineering, and technology. BES has been a leader in the early development of this work since the 1980s, supporting research and sponsoring workshops to help establish the importance of nanostructured materials. BES is currently making a broad range of contributions in areas such as the enhanced properties of nanocrystals for novel catalysts, tailored light emission and propagation, nanocomposites, and supercapacitors. Nanocrystals and layered structures offer unique opportunities for tailoring the optical, magnetic, electronic, mechanical, and chemical properties of materials, and layered structures have already been synthesized for electronics, novel magnets, and surfaces with tailored hardness. Examples of research already supported by BES include:

- *Addition of aluminum oxide nanoparticles that convert aluminum metal into a material with wear resistance equal to that of the best bearing steel*
- *Novel optical properties of semiconducting nanocrystals that are used to label and track molecular processes in living cells*
- *Nanoscale layered materials that can yield a four-fold increase in the performance of permanent magnets*
- *Layered quantum well structures to produce highly efficient, low-power light sources and photovoltaic cells*
- *Novel chemical properties of nanocrystals that show promise as photocatalysts to speed the breakdown of toxic wastes*
- *Meso-porous inorganic hosts with self-assembled organic monolayers that are used to trap and remove heavy metals from the environment*

In addition, BES supports a truly impressive array of major national user facilities that are ideally suited to visualizing, characterizing, and controlling the nanoworld – from atoms and molecules to bulk materials. The four synchrotron radiation light sources, three neutron scattering facilities, and four electron beam microcharacterization centers operated by BES together represent the largest collection of such facilities in the world operated by a single organization. Thus, with its large portfolio of fundamental research and with its support for major national user facilities, BES is in a unique position to make major contributions to the NNI.

This work will benefit missions throughout the Department of Energy. Nanoscale synthesis and assembly methods will result in: significant improvements in solar energy conversion; more energy-efficient lighting; stronger, lighter materials that will improve efficiency in transportation; greatly improved chemical and biological sensing; use of low-energy chemical pathways to break down toxic substances for environmental remediation and restoration; and better sensors and controls to increase efficiency in manufacturing.

The BES program has worked with the National Science and Technology Council's Interagency Working Group on Nanotechnology, with the Basic Energy Sciences Advisory Committee (BESAC), and with the broad scientific community from academia, industry, and the national laboratories to define and articulate the goals of this research and to determine how best to implement a program of research. Two recent reports prepared by the BES program, which address both NSET research and broader program goals that are dependent on nanoscale understanding, are available on the internet. These reports are *Nanoscale Science, Engineering and Technology Research Directions* (1999) available at http://www.er.doe.gov/production/bes/nanoscale.html, and *Complex Systems: Science for the 21st Century* (1999) available at http://www.er.doe.gov/production/bes/complexsystems.htm.

The BES program in NSET has the following overarching goals: (1) attain a fundamental scientific understanding of nanoscale phenomena, particularly collective phenomena; (2) achieve the ability to design and synthesize materials at the atomic level to produce materials with desired properties and functions; (3) attain a fundamental understanding of the processes by which living organisms create materials and functional complexes to serve as a guide and a benchmark by which to measure our progress in synthetic design and synthesis; and (4) develop experimental characterization tools and theory/modeling/simulation tools necessary to drive the nanoscale revolution.

The first goal of this work is the fundamental scientific understanding of structures and interactions at the nanoscale, particularly collective phenomena. It is known that when sample size, grain size, or domain size shrink to the nanoscale, physical properties are strongly affected and may differ dramatically from the corresponding properties in the bulk. Yet, there is remarkably little experience with phenomena at the nanoscale. Because of this limited experience, the physical and chemical properties of nanoscale systems are not understood. In effect, this is a new subject with its own set of physical principles, theoretical descriptions, and experimental techniques. One of the most interesting aspects of materials at the nanoscale involves properties dominated by collective phenomena -- phenomena that emerge from the interactions of the components of the material and whose behavior thus differs significantly from the behavior of those individual components. In some case, collective phenomena can bring about a large response to a small stimulus -- as seen with colossal magnetoresistance, the basis of a new generation of recording memory material. Collective phenomena are also at the core of the mysteries of such materials as the high-temperature superconductors, one of the great outstanding problems in condensed matter physics.

The second goal of this work -- the design and synthesis of materials at the atomic level for desired properties and functions -- is the heart of nanoscale science, engineering, and technology. In the future, design and synthesis of new materials at the atomic level will be accomplished using only the electronic structure of the elements. Theory, modeling, computational

simulation, and experiment all play critical roles in this quest. Because of the small dimensions, it will be possible in many cases to calculate the desired properties of materials knowing only the atoms that make the material. In cases where simulation is not possible, powerful experimental combinatorial approaches can be used to vary conditions and compositions and search for materials with new or improved properties. Large numbers of differing samples can be made and tested very quickly. These experimental approaches will be especially important for structures that are not at equilibrium, that might include small amounts of minor constituents, and that might be prepared using extreme conditions such as high pressure or high magnetic fields. A very important part of the research for this goal is the synthesis of molecular building blocks that will lead to functional materials and the design of molecular machines from molecular building blocks.

The third goal of this work is the fundamental understanding of the processes by which living organisms create materials and functional complexes. Nanoscale science, engineering, and technology inexorably links the physical and biological sciences. Nature arranges atoms and molecules precisely into three-dimensional objects of extraordinary complexity to produce objects with required optical, mechanical, electrical, catalytic, and tribological properties. Nature has also learned how to combine materials and structures to build molecular-level machines. Some of these molecular machines serve as pumps, moving material across barriers; others move molecules, structures, or whole cells; others control processes and thus are regulatory systems; and still others produce or convert energy. A major challenge in the physical sciences is to understand how Nature makes these complex objects and molecular machines so that we can develop the tools to design and build materials that function as we want -- materials that have not been envisioned by Mother Nature but use Nature's self assembly techniques. By understanding and applying these principles to artificial systems, we can make potentially immense advances in diverse areas including energy conversion; data transmission, processing, and storage; "smart" and adaptable materials; sensors for industrial, environmental, and defense purposes; new catalysts; better drugs; and more efficient waste disposal.

The fourth goal of this work is the development of experimental characterization tools and theory/modeling/simulation tools. The history of science has shown that new tools drive scientific revolutions. They allow the discovery of phenomena not previously seen and the study of known phenomena at shorter time scales, at shorter distances, and with greater sensitivity. The BES program has been a leader in the development of tools for characterization at the nanoscale. Required new instrumentation will necessarily involve an enhancement of conventional techniques -- scanning-probe microscopies, steady-state and time-resolved spectroscopies, and so forth. However, characterization will also depend heavily on revolutionary experimental tools, including techniques for the active control of growth, for massively parallel analysis, and for small sample volumes. Capabilities will be needed for triggering, isolating, or activating single molecules; for independently addressing multiple molecules in parallel; and for transferring or harvesting energy to or from a single molecule. New generations of theory and computational tools will also be required.

b. Investment Strategy

Overview. Research in NSET involves materials sciences, chemistry, physics, biology, and computation. Based on community interactions and on recent recommendations from BESAC, the BES program will establish a portfolio of activities balanced in scope and in size, ranging from

individual principal investigators to large groups. Proposals will be encouraged from individual investigators, from relatively small groups of a few principal investigators at universities and/or national laboratories, and from larger groups focused on particular problems such as might be appropriate for a university center, a national laboratory, or a user facility. Interactions among scientists with a diverse set of skills in areas such as molecular design, synthesis and assembly, molecular modeling, instrumentation development, theory and modeling, and device engineering will be encouraged. Involvement of young investigators -- graduate students, postdoctoral research associates, and young facility and staff -- with appropriate expertise is critical to the success of the science and to the evolving future of this field. Few researchers are now trained in the multidisciplinary aspects of the work that will be required to achieve the goals of the program. Interactions among several institutions, including both academic and national laboratory partners, is expected to occur naturally for each of the major focus areas.

FY 2001 Request. In the FY 2001 request, new funding in the amount $36.1 M is requested for these activities in BES, an increase of 77 percent over the FY 2000 BES investments of $47.0 M in these areas. New funds are distributed within the Materials Sciences (18.3 million), Chemical Sciences ($12.8 million), and Engineering and Geosciences ($5.0 M) subprograms. Contained within these amounts are funds specifically addressing facilities operation and enhancements ($3.2 M) and theory, modeling, and computation related to problems in NSET ($5.6 M).

Specific focus areas within each of the subprograms are described in detail in the subprogram narratives within the BES budget, which is available at http://www.er.doe.gov/production/bes/budget.html. Within the Materials Sciences subprogram, investments will be in the areas of structure of materials, engineering behavior of materials, experimental and theoretical condensed matter physics, materials chemistry, and facilities operation. Within the Chemical Sciences subprogram, investments will be in the areas of atomic, molecular, and optical sciences; chemical physics; photochemistry and radiation research; catalysis and chemical transformations; separations and analysis; heavy element chemistry; chemical engineering; and facilities operations. New funding in these disciplinary areas must address the four broad goals described above. All awards will be made based on a competitive peer review process following announcements to universities and DOE laboratories for proposals in areas described in this paragraph.

The BES Program in the Context of the NNI Interagency Effort. The NNI initially supports activities in the five areas: (a) Long-term fundamental nanoscience and engineering research, (b) Grand Challenges in areas such as nanostructured materials by design - stronger, lighter, harder, self-repairing, and safer; nanoelectronics, optoelectronics and magnetics; nanoscale processes for environmental improvement; efficient energy conversion and storage; and bio-nanosensors; (c) Centers and Networks of Excellence, (d) Research Infrastructures for metrology, instrumentation, modeling and simulation, and user facilities, and (e) Ethical, Legal, Societal Implications and Workforce Education and Training.

The BES contribution to these areas provides approximately +$3 M for research infrastructure and nearly equal amounts for fundamental research (approximately +$16 M) and grand challenges (approximately +$17M). The latter will be concentrated in the areas described above, which is only a partial list of the NNI grand challenge areas. The grand challenge areas chosen for emphasis by BES are those that underpin the mission of the DOE.

D4. Department of Transportation (DOT)

a. Background

"Economical and safe transportation" through the adoption of novel materials, electronics, energy conversion and storage technologies, and security concepts is among the "grand challenges" of the NNI. Although the Department has not requested funding for the NNI for FY-2001, the Department must be able to fund explicitly transportation-related R&D to fully capture nanotechnology's benefits.

b. Investment Strategy

Plans to support the NNI in FY 2002 and beyond include (1) support for a broad program of university research and education, and (2) targeted research to expedite the development of promising nanotechnology applications. Specific programs may include:

University Consortia Program: Following a "technology scan" to identify which applications of nanotechnology would have the greatest payoff for transportation, DOT may establish a cost-shared University Consortia Nanotechnology Research and Applications Program. The program would support broad-based consortia for research and education in promising nanotechnology application areas. Modeled after the DOT/NASA Commercial Remote Sensing program, this effort would fund five or six consortia, or "virtual centers," among the University Transportation Centers (UTCs) and other agencies' Centers of Excellence in nanotechnology. Each consortium would focus on a key application area. A joint panel of experts from the DOT modes and other agencies would review the proposals and select the consortia teams. Program management and oversight would be shared with these agencies through Memoranda of Understanding. As part of this program, DOT also would conduct outreach to States, local agencies, and the transportation industry to inform them of relevant nanotechnology research and developments.

***Nanotechnology Applications to Highways*:** Currently, Portland cement and asphalt concrete mix designs are developed on a trial and error basis, making it difficult to achieve specified performance. Rational concrete design requires fundamental knowledge on the nanometer scale at which the materials properties are determined. To this end, DOT may pursue a targeted research program to apply nanoscale measurement methods to characterize development of microstructure; develop advanced computer models of microstructure growth; apply models to improved materials processing; apply MEMS sensors with nanotechnology components to monitor nanostructure development and structural performance; develop better energy dissipative materials for roadside safety structures; and apply MEMS sensors with nanotechnology components to monitor the dynamic and kinematic environment of an impacted roadside safety structure.

***Nanotechnology Applications to Aviation Security*:** Research in nanotechnology and MEMS with nanotechnology components is critically needed to improve the detection of trace/bulk explosives and of both chemical and biological weapons. Toward this end, DOT may apply novel chemical detectors based on nanotechnology and MEMS integrated circuits to sense trace levels of explosives and chemical/biological weapons at checkpoints and in checked bags; investigate nano detection (building on current research in "nanoexplosion"/ detection with microcantilever surfaces) with

MEMS remote receive/transmit systems embedded on the chip; study monolayer and cluster nanolayers of selective polymers on surfaces to selectively collect, preconcentrate and detect trace levels of explosives and other hazards; and characterize molecular detection mechanisms to investigate novel miniature inlet/preconcentrator systems (with MEMS) for enhanced sensitivity and selectivity.

Nanotechnology Applications to Rail: To expedite applications to rail transportation, DOT may conduct outreach with nanotechnology researchers and the rail industry to identify applications that hold the most promise (e.g., sensors that continuously monitor rail infrastructure performance, corrosion-resistant coatings and materials, self-extinguishing materials) and disseminate the results of relevant nanotechnology research to the rail industry.

D5. National Aeronautics and Space Administration (NASA)

a. Background

Program planning and Implementation Approach. NASA will typically use open solicitations and peer-reviewed competition for allocating basic research funds. Coherent, applications-oriented development programs with strong NASA Center participation will be established to address specific grand challenges. The selection of challenges to address will be aligned with science priorities of the agency enterprises. NASA will also seek external scientific, engineering and biomedical expertise in determining the technical content of the program, and in reviewing the progress of the work to ensure quality. Opportunities will be sought with university research centers to arrange for student and postdoc participation in NASA's grand challenge research, including opportunities to work for periods of time at NASA Centers.

Opportunities for Collaboration with other Agencies. Collaboration is particularly important for NASA, given its relatively modest investment in nanotechnology. A joint program in imaging and characterization at the molecular level is currently being developed with NIH/NCI based on common interests in this area. Other potential areas for collaboration are:

Area of Common Interest	Potential Agency Collaborators
Aerospace structural materials	DOD
Radiation tolerant devices and materials	DOD
Biosensors, lab-on-a-chip, environmental monitoring	DOE, DOD, NIH
Targeted therapeutic delivery	NIH
Exploratory computational architectures	DOD, NSF
Micro spacecraft systems	DOD
Efficient energy conversion and storage	DOE
Basic research in nanostructures	NSF

Opportunities for Private Sector & International Collaboration. NASA has an ongoing program with Rice University with a focus on applications of carbon nanotubes to aerospace vehicle structures, batteries and energy storage, and nano devices. A number of other universities are

involved in various aspects of the ongoing nanotechnology work. National collaboration opportunities of potential mutual benefit include:

Area of Common Interest	Potential Collaborators
Bionanotechnology, nanostructured materials, nanodevices, exploratory computational architectures	Universities
Microspacecraft technologies	Small and large aerospace industry
Biochips	Biotechnology industry

NASA's interaction with international activities is typically in international space missions, which are negotiated among the space agencies of the collaborating nations, and are implemented with no exchange of funds. This approach permits the international science community to benefit from technology and infrastructure investment around the world.

b. Investment Strategy

For FY 2001, NASA's commitment to nanotechnology is $20M, of which $5M represents ongoing programs, and $15M will support new work. The existing work resides primarily in the Cross Enterprise Technology Development Program, the SBIR Program and NASA Center internal discretionary programs. The new work resides in 2 new programs:

1. $10M will be implemented in the new Bioastronautics Program within the Human Exploration and Development of Space Enterprise. Of this, $5M is part of the Bioastronautics base program, and $5M represents part of a new $10 M program to be implemented in partnership with NIH/NCI.
2. $5M will be implemented as a new activity in the Space Science Enterprise.

Fundamental Research. NASA looks to NSF-sponsored work for wide-ranging contributions in fundamental research, and expects to allocate only a modest portion (10-20%) if its program to basic research, emphasizing work in direct support of the grand challenge areas the agency selects for focus. *Grand Challenges.* NASA expects to allocate the majority (50-60%) of its nanotechnology program funds to address priority challenges of future robotic and human aerospace systems. In addition to specific overlap in applications requirements with various government agencies, NASA expects to leverage the nation's investment in basic research as starting points for much of its investment in applications-oriented grand challenges, including the following specific areas within the grand challenge areas:

<u>Nanostructured Materials "By Design".</u>
NASA's focus in this area is on high strength-to-mass, "smart" structural materials in the context of

- Safer, more reliable, multifunctional and eventually self-repairing aerospace vehicle structures
- Truly smart and agile materials with programmable optical, thermal and/or mechanical properties
- High-precision, low-mass, very-large optical elements with active surface figure control, and self-cleaning surface finishes
- Ultra-large space structures such as antennas, solar sails and gossamer spacecraft
- Materials for special environments, e.g. low/high temperature, low/high pressure, low/high gravity, high radiation and chemically reactive

DOD has overlapping interests in large space optics and antennas, and high-strength-to-mass aerospace structural materials in general. A joint program already exists in gossamer space structures, which will consider options based on nanostructured materials.

Nano-Electronics, Optoelectronics and Magnetics

Priority areas for NASA are in nanoscale devices and novel computational architectures for

- Quantum-limited sensors of electromagnetic radiation and fields, able to capture multiparameter information in detecting single quanta
- Low-power, ultra-high-speed signal processing devices and computers
- High-density, radiation-tolerant memory technologies
- Devices for special environments, e.g. low/high temperature, low/high pressure, low/high gravity, high radiation and chemically reactive

DOD has overlapping interest in radiation tolerant devices and new architectures for ultra-high-speed space-based computing.

Advanced Healthcare, Therapeutics and Diagnostics

The challenge of ensuring astronaut health and performance, drives NASA to a focus on biochemical signatures of incipient problems, and on nanoscale in vivo, and minimally invasive biochemical sensors and therapy effectors in the context of

- Early detection of incipient health and performance problems of astronauts
- Targeting and delivery of preventative and curative therapeutics
- In situ detection and characterization of life beyond Earth's biosphere

There is strong overlap with NIH in this area, and a joint program is being planned with NIH/NCI in the general area of detection and imaging at the molecular level. There is also overlap with biosensor development outside of the medical arena in DOD and DOE covered under the Bio-Nanosensor category, below.

Efficient Energy Conversion and Storage

NASA is interested in high-efficiency, low-mass solar and thermal energy conversion for space power, high-mass-efficiency power storage and distribution, and efficient low-temperature refrigeration for ultra-sensitive space-based sensors. DOE shares the goals of high-efficiency energy conversion and storage.

Microspacecraft Space Exploration and Industrialization

NASA's focus in this area is on low-mass, low-power, devices, subsystems and systems with the following goals:

- Reduction in size and energy consumption of capable spacecraft by a factor of 10
- Greatly increased on-board capability for signal processing, real-time decision making and autonomy

- Low-power, miniature spacecraft systems including sensors, signal processing, avionics, inertial guidance, propulsion and communications
- Bio-mimetic evolvable space system architectures that can adapt to new environments and mission needs, and eventually to self-replicate using local resources at distant locations

There is overlap with microspacecraft goals of DOD, and cooperative programs will be considered.

<u>Bio-Nanosensor Devices for Communicable Disease and Biological Threat Detection</u>
NASA's focus in this area is on nanoscale sensors and integrated laboratories for the purpose of monitoring and controlling human space habitat environments. Agencies with overlapping interests are DOD (detection of biochem-warfare agents), DOE (lab-on-a-chip for detecting environmental pollutants and biological threats).

<u>Economical and Safe Air Transportation</u>
NASA's focus in this area is on smart materials and advanced aircraft avionics for

- Economical air, Earth-to-orbit and deep-space transportation based on more reliable materials, smart systems for condition-based maintenance, and lower overall mass

Agencies with overlapping interests are DOD (low-cost air and space transportation), DOC (low-cost air transportation).

Research Infrastructure. Investment in research infrastructure is allocated 20 - 30% of NASA's nanotechnology budget for FY 2001. The primary areas of focus are in support of the delineated grand challenges:

a. The development of measurement instrumentation for imaging and characterizing nanostructures being developed under NASA's grand challenge categories

b. Tools for modeling and simulation of relevant mechanical, thermal, optical and electronic properties of nanostructures and systems

D6. National Institutes of Health (NIH)

a. Background

NIH will support nanotechnology research that has exceptional promise to lead to new materials and tools for the diagnosis and prevention of disease, novel therapeutic solutions, and enhanced methods for conducting laboratory, clinical, behavioral and population research. Very little is known today about how to harness the rudimentary concepts and tools developed by nanotechnologists from other disciplines, for uses in biology and medicine. It is probably true that the most important ways in which nanotechnology will ultimately contribute to biomedicine cannot even be foreseen today. Through solicitations that promote new research ideas that are firmly grounded in the best science, NIH will encourage applications to leverage the essential new knowledge that will be generated largely through the support of other agencies that are cooperating in this initiative. Even though many of the ultimate uses of nanotechnology for medicine cannot be predicted, we have a basis, from more evolutionary developments, to envision some near-term

(five-to-ten years from realization) applications. These include sensors for the early detection of disease, materials and strategies for dispensing therapeutic agents in ways that enhance desired effects while minimizing adverse side effects, new materials to repair and replace parts of the body damaged by age and disease, and increasingly sensitive and novel measuring tools to study biomolecular systems in their native states.

*Research support through peer reviewed grants to achieve NNI goals***.** At the NIH, this research will be supported for the most part through peer-reviewed grant applications submitted by individual investigators and groups of investigators, and to a lesser extend through intramural NIH laboratories. To stimulate investigators to develop new research programs in nanotechnology, NIH has already published two announcements. One requests applications using the SBIR mechanism. The second lists several existing grant programs under which nanotechnology research projects may be supported. In particular, the Bioengineering Research Partnerships program, organized by the NIH Bioengineering Consortium (BECON) with broad participation by the NIH Institutes and Centers, offers the opportunity for investigators from diverse scientific, clinical and engineering fields, in academia, national laboratories, and industry, to assemble the interdisciplinary teams required for much of this research.

Thus, NIH has in place mechanisms to support fundamental research and projects to meet grand challenges for the solution to specific biomedical problems, through individual laboratory and "centers" scale projects. NIH will support the infrastructure needed to accomplish the research goals of these projects, through (a) including in project budgets the funds needed to purchase equipment and services appropriate to the scale of the project, (b) funding of user fees at national or regional facilities, and (3) infrastructure grants (e.g., through NCRR). NIH also has in place several programs to support an additional prong of the NNI strategy, namely training and workplace issues. Several of the Institutes and Centers have in place programs to support the training of scientists and engineers at many career levels, from pre-doctoral to professional, in the cross-disciplinary environments that are needed to facilitate the incorporation of new technologies and approaches into biomedicine. The training needed to enable nanotechnology research falls squarely into several of these programs. One specific example is the Mentored Quantitative Research Career Development Award program, initiated last year through the efforts of BECON and with cooperation from most of the NIH IC's.

Obtaining expert advice from external sources, for programs and expenditure of federal funds. The advice of a broad cross-section of the research community on the potential importance of nanotechnology, on fruitful research pathways, and on the projects that are worthy of federal support, is obtained through well-established mechanisms.

1. For example, the NIH Bioengineering Consortium (BECON) will host a seminar in June 2000 to inform biomedical researchers about this exciting field of nanotechnology, identify applications of nanotechnology that are relevant to biology and medicine, and explore future research possibilities to ensure that the NIH is poised to effectively facilitate biomedical research incorporating nanotechnology concepts. Attendance is expected by 500 extramural and intramural biomedical scientists, clinicians, and nano scientists from the physics, chemistry, computational, mathematics, and engineering communities. Attendees will have the opportunity to contribute to the meeting report, which will serve as a guide to NIH for near-future funding

initiatives and program management. It is anticipated that individual programs at the level of institutes, or consortia of institutes, will host future conferences as the field evolves.

2. For the funding of individual project grants, the peer-review of grant applications is a primary and essential component of the process for selecting projects to receive federal funds. The NIH review process is highly effective, but ways to improve it continue to be sought, such as the inclusion of scientists, clinicians, and engineers with broader views and expertise, and receptiveness to projects designed to develop new technologies.

3. The Advisory Councils of individual Institutes and Centers, comprised of individuals highly respected for their scientific expertise and judgment, and their contributions to other endeavors related to healthcare and delivery, must review and approve new solicitations issued by the IC's. The purpose of this review is to ensure an appropriate balance among the possible uses of the Institutes' funds for exploring novel and substantial means to achieve Institute goals.

b. Investment strategy

The NNI plus-up for NIH is modest. However it is anticipated that the growing awareness of the potential impact available from investment in nanoscience, engineering and technology at the NIH Institutes will lead to significant investment from core funds.

Portfolio management and coordination. Each of the funding components will manage its own portfolio of nanotechnology projects, to meet the needs of each of the independently funded Institutes' and Centers' missions. Coordination across the NIH will occur through BECON, which already serves as a focal point for bioengineering and technology development-related issues. Other trans-NIH working groups will also play a role in coordinating nanotechnology research strategies under their purview. For example, the existing Biomaterials and Medical Implant Science (BMIS) Coordinating Committee will be intensively involved in monitoring and proposing new directions for nanotechnology research to develop new materials and strategies for implantable devices.

NIH maintains active liaison to other government agencies involved in NNI (i.e. DOE, NSF, NIST, NASA, DOD) through BECON and other trans-NIH working groups, and through specific programs within the Institutes and Centers. Representatives to two of the NNI agencies are participating members of BECON and two BECON members are NIH representatives to the NSET. Frequently, the representatives to other trans-NIH initiatives are also BECON members (for example, many BMIS members are also the representatives from their IC's to BECON, and similarly, IC reps to other agencies or industry for institute-specific initiatives often are, or work closely with, their IC's reps to BECON because their grant portfolios are closely related). Through these active liaisons, NIH staff and our colleagues from other agencies seek opportunities to collaborate or fill gaps between programs, when it is perceived that existing mechanisms fail to stimulate or optimally support the research that is needed to achieve agency missions.

Most of the synergy that occurs when multiple agencies fund the research that occurs at a particular grantee institution, or even within a particular scientist's laboratory, occur because good scientists and engineers have many ideas and can use their knowledge to serve the missions of multiple

agencies. It is a strength of our federal funding system that the approaches to decision making and goal setting are diverse, serving well the diversity of research that is needed. It is important to maintain this diversity and not “over-manage” programs, such as the NNI, which could result in too singular an approach. However, sometimes scientists within the agencies can identify potential collaborations, and resources that can be more effectively leveraged, and when that occurs the science can be advanced. Some NIH components have initiated such activities in recent years for nanotechnology, and opportunities to identify additional ones will continue to be sought. For example, the NCI and DARPA co-funded some grants whose goals served the missions of both agencies, and NCI issued a contract to NASA-Ames lab for research that leveraged NASA capabilities to serve the NCI mission.

The NIH BECON recently reorganized its web pages to better serve the grantee community and public. Each of the NNI participant agencies is working to link together useful information about its nanotechnology programs. One outcome will be that grantees and potential applicants will have well-organized information sources on the resources and expertise that are available to support nanotechnology research. Establishment of this information network will speed scientific discovery and reduce duplication of effort.

D7. National Science Foundation (NSF)

a. Background

"Nanoscale Science and Engineering" is the NSF contribution to the **National Nanotechnology Initiative – Leading to the Next Industrial Revolution (NNI)** recommended by the Administration for FY2001. Nanotechnology is the creation and utilization of functional materials, devices and systems with novel properties and functions that are achieved through the control of matter atom by atom, or molecule by molecule, on a scale of a fraction of a nanometer to tens of nanometers. A revolution has begun in science, engineering and technology, based on the ability to organize, characterize, and manipulate matter systematically at the atomic and molecular level. Far-reaching outcomes for the 21st century are envisioned on both scientific knowledge and a wide range of technologies in most industries, healthcare, conservation of materials and energy, biology, environment and education. Nanoscience and engineering underpins innovation in critical areas ranging from information technology, biotechnology and medicine on one side to materials, manufacturing and environment on the other side.

Formidable challenges remain, however, in the areas of fundamental understanding, device design, manufacturing, and systems-level integration and deployment before the potential of nanotechnology becomes a reality. NNI will ensure that investments in this area are made in a coordinated and timely manner, and will accelerate the pace of revolutionary discoveries now occurring in nanoscience and engineering. A window of opportunities has opened as new tools allow for fundamental discoveries and technology use. Initial applications have proven outstanding benefits.

NSF has established the Nanoscale Science and Engineering Committee, with representatives from all research and education directorates (BIO, CISE, ENG, EHR, GEO, MPS and SBE).

Long-term Strategy. NSF has been a pioneer in fostering the development of nanoscience and engineering. NSF investment is approximately $97 million in FY 2000 in a wide range of research and education activities. NSF's thrust will form part of the inter-agency NNI effort planned for FY 2001, with the goals of creating a vigorous, interdisciplinary activity for fundamental research and education in nanoscience and engineering, establishing an appropriate physical infrastructure and developing the workforce needed to exploit the opportunities presented by these new capabilities.

The long-term objectives of NNI are: (1) expedite long-term, fundamental research aimed at discovering novel phenomena, processes and tools, including nanoscale systems that are important in computing, biology and in the environment, (2) address the synthesis and processing of engineered, nanometer-scale building blocks for materials and system components, (3) develop new device concepts and system architecture appropriate to the unique features and demands of nanoscale science and engineering, (4) apply nanostructured materials to innovative technologies for commerce (manufacturing, computing and communications, power systems, energy), health, the environment, and national security, and (5) Ethical, legal, societal implications and workforce education and training of a new generation of skilled workers in the multidisciplinary perspectives necessary for rapid progress in nanotechnology.

During the next five years, NSF will emphasize research investment on five inter-related areas at the frontiers of nanoscale science and engineering: (a) biosystems at the nanoscale, (b) nanoscale structures and quantum control, (c) device and system architecture, (d) environmental nanoscale processes, (e) theory, modeling and simulation, and (f) societal and educational impact of scientific and technological advances on the nanoscale. To stimulate creativity, cross-fertilization of fields, and invention with potential impact beyond that of the current effort, support will be focused on interdisciplinary research teams, nanoscale science and engineering centers, academic partnerships with industry and national laboratories, and on exploratory research projects.

b. Investment Strategy

NSF's planned investment for NNI in FY 2001 is $216.7 million. Participating directorates include the Biological Sciences with $4.90 million, Computer and Information Sciences and Engineering with $5 million, Engineering with $87.50 million, Directorate for Geosciences with $7.84 million, and Mathematical and Physical Sciences with $111.41 million. This level of investment will strengthen critical fields and help to establish the science and engineering infrastructure and workforce needed to exploit the opportunities presented by these new capabilities.

In FY 2001, NSF will emphasize research and education in five programmatic activities:

<u>Fundamental research at nanoscale</u>. The request of $122 million in FY 2001 ($65 million over FY 2000) will fund single investigators and small groups with awards typically for three to five years. The following interrelated topics will be emphasized:

- *Biosystems at the Nanoscale ($20 million)*. Research in this area supports the development of a fundamental understanding of nanobiostructures and processes, nanobiotechnology, and techniques for a broad range of applications in biomaterials, biosystem-based electronics,

agriculture, energy, and health. The goal is to stimulate progress in the study of biological and biologically inspired systems in which nanostructures play an important role. This includes developing an understanding of the relationships among chemical composition, physical shape and biological function. Biosynthesis and bioprocessing offer fundamentally new ways to manufacture nanostructured products, including novel biomaterials, improved drug or gene delivery, nanoscale sensory systems, biochips, and the modification of existing biomolecular machines for new functions.

- *Nanoscale Structures, Novel Phenomena, and Quantum Control ($45 million)* - Research in this area explores the novel phenomena and structures that appear at the nanoscale. This research is critical to overcoming obstacles to miniaturization as feature sizes in devices reach the nanoscale. Research in this area also refers to development of the experimental tools necessary to measure nanostructures and phenomena, and development of techniques for synthesis and design. Examples of possible applications include molecular electronics, quantum computing, DNA computing, the development of high capacity computer memory chips, production of two- and three-dimensional nanostructures "by design", as well as investigations of quantum algorithms and means for error correction in quantum information systems.
- *Device and System Architecture ($27 million)* – New concepts are needed to understand interactions among nanoscale devices in systems, the design of nanoscale systems, and their integration into architectures for various operational environments. Collaborative research among physicists, chemists, biologists, material scientists, computer scientists and engineers will be necessary. Research in this area includes development of new tools for sensing, assembling, processing and manipulation of nanostructures, devices and architectures, and design automation tools for architectonic assemblies of large numbers of heterogeneous nanocomponents. One can envision "smart" systems that sense and gather information and analyze and respond to it (for monitoring health for example), and more powerful computing structures and architectures.
- *Nanoscale Processes in the Environment ($15 million)* - Research in this area will focus on probing nanostructures and processes of relevance in the environment from the Earth's core to the upper atmosphere and beyond. Emphasis will be on understanding the distribution, composition, origin, and behavior of nanoscale structures under a wide variety of naturally occurring physical/chemical conditions, including nanoscale interactions at the interface between organic and inorganic solids, liquid and gases, and between living and non-living systems. This research area also includes biomineralization of nanoscale structures, development of environmental biotechnology, study of transport of ultrafine colloidal particles and aerosols, and study of interplanetary dust particles. Examples of possible applications include better understanding of molecular processes in the environment, the development of manufacturing processes that reduce pollution, and new water purification techniques and artificial photosynthetic processes for clean energy.
- *Multi-scale, Multi-phenomena Modeling and Simulation at Nanoscale ($15 million)* - The emergence of new behaviors and processes in nanostructures, nanodevices and nanosystems creates an urgent need for theory, modeling, large-scale computer simulation and design tools and infrastructure in order to understand, control and accelerate the development in new nanoscale regimes and systems. Research on theory, modeling and simulation of physical, chemical and biological systems at the nanoscale may include techniques such as quantum mechanics and quantum chemistry, multi-particle simulation, molecular simulation, grain and continuum-based models, stochastic methods, and nanomechanics.

Grand challenges. The FY 2001 request of $12 million ($9 million over FY 2000) will fund interdisciplinary research and education teams that work on major, long-term objectives: nanostructured materials 'by design', nanoscale-based manufacturing, nano-electronics, optoelectronics and magnetics, environment and healthcare.

Centers and networks of excellence. FY 2001 funding at $37 million ($21 million over FY 2000) will provide support for new centers, research networking and shared academic user facilities. Centers will play an important role in fundamental research, grand challenges and education, in development and utilization of the specific tools, and in promoting partnerships in the next decade.

Research infrastructure. FY2001 funding at $24.7 million (12.7 million over FY 2000) will support instrumentation and facilities for improved measurements, processing and manipulation at nanoscale, and equipment and software for modeling and simulation. It will encourage university-industry-national laboratory and international collaborations particularly for expensive instrumentation and facilities.

Societal and Education Impact of Scientific and Technological Advances on the Nanoscale. FY 2001 funding at $21 million ($12 million over FY 2000) will support student fellowships and traineeships, curriculum development on nanoscience and engineering, and for developing new teaching tools, as well as studies on the impact of nanotechnology on society from legal, ethical, social, economic and workforce perspectives. Exploitation of scientific and engineering advances at the nanoscale will bring along with it expected and sometimes unexpected impacts on society. The development and use of nanoscale technologies is likely to change the design, production and use of many goods and services, ranging from vaccines to computers to automobile tires. Studies might include (not exhaustive): economic assessments of the lifecycle of nanoscale development and use; business models for nanotechnology; how the public understands nanoscience and technology; the ethical and legal ramifications of nanotechnology in health, medicine, law, and the environment; knowledge barriers around the adoption of nanotechnology by commercial firms; an understanding of its diffusion patterns; and the implications of nanotechnology for everyday life.

About 67% of awards will be made in open competition in the broad-based NSF programs. A FY 2001 NSF-wide initiative will invest about 33% of the funds on interdisciplinary small-group proposals, centers and networks of excellence in nanoscale science and technology. The focus will on activities that have an added value as compared to the disciplinary programs; we will involve the existing programs without establishing parallel paths with the existing program structures.

Related NSF NNI Activities. NSF currently invests in a wide range of research activities in nanoscale science and technology, including the five nanotechnology research hubs with a focus on electronics, biology and optoelectronics. Research and education in this area is supported through individual investigator awards, small groups, centers (MRSECs, STCs, ERCs), instrumentation, and facilities such as the NNUN. The support is distributed across several directorates and spans many disciplines. NSF supported a cross-directorate initiative "Partnership in Nanotechnology: Functional Nanostructures" in FY 1998, focused SBIR/STTR announcements on nanotechnology in FY 1999, and "Exploratory Research on Biosystems at Nanoscale" and "Nanoscale Modeling and Simulation" in FY 2000.

Interagency NNI Activities. The NSET is coordinating individual agencies' activities to identify research directions, coordinate funding activities of centers and networks of excellence, and the development of partnerships. Opportunities for collaborative activities identified with other agencies in FY 2001 include research on molecular electronics and spin electronics (with DOD), advanced materials, nanoscale modeling and simulation (a special emphasis with DOD), devices and system architectures, bioengineering (with NIH), laboratory on a chip, quantum computing (with NASA and DOD), and use of university-based and National Laboratory-based user facilities for advanced tools and manipulation at the nanoscale.

Longer-term objectives (in FYs 2001-2005):

- Research – fund the core scientific and engineering challenges and provide the generic foundation for Grand Challenges
- Infrastructure – ensure that 50% of research institutions will have access to a full range of nano-facilities
- Education – enable education access to nanotechnology for at least 50% of all students in research universities
- Catalyze the creation of at least three new commercial markets that depends on 3-D nano-structures